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User's Manual for TOX-SCREEN:

A Multimedia Screening-Level Program for Assessing the Potential Fate of Chemicals Released to the Environment

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The purpose of this report is to provide a user's manual for the FORTRAN IV computer code, TOX-SCREEN, which implements the multimedia model. A brief description of the model assumptions and structure is included. The structure of the TOX-SCREEN program and individual subroutines are described in detail. Input to and output from the code are thoroughly explained. Parameter definitions, sample job control language, sample input data, output from TOX-SCREEN using the sample input data, and a listing of the program are provided in appendixes.

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ABSTRACT

A screening-level multimedia model called TOX-SCREEN has been developed to assess the potential fate of toxic chemicals released to air, surface water, or soil. Four types of surface water bodies are considered: lakes, rivers, estuaries, and oceans. TOX-SCREEN was developed at the request of the U.S. Environmental Protection Agency (USEPA) to provide a means by which chemicals classified under Section 4 of the Toxic Substances Control Act (TSCA) can be rapidly evaluated with respect to their potential for accumulation in environmental media. The model is simplified in nature and is intended to be used as a screening device to identify chemicals that are unlikely to pose problems even under conservative assumptions.

The purpose of this report is to provide a user's manual for the FORTRAN IV computer code, TOX-SCREEN, which implements the multimedia model. A brief description of the model assumptions and structure is included. The structure of the TOX-SCREEN program and individual subroutines are described in detail. Input to and output from the code are thoroughly explained. Parameter definitions, sample job control language, sample input data, output from TOX-SCREEN using the sample input data, and a listing of the program are provided in appendixes. Also, methods for estimating bioaccumulation in food chains, added recently to TOX-SCREEN, are documented in an appendix.

1. INTRODUCTION

A screening-level multimedia model has been developed to assess the potential for human exposure to chemicals released to air, surface water, or soil. This model was developed at the request of the U.S. Environmental Protection Agency (USEPA), Office of Toxic Substances, as a part of their endeavor to fulfill regulatory responsibilities under the Toxic Substances Control Act of 1976. A document describing the model assumptions, mathematical structure, and overall framework was recently published (McDowell-Boyer and Hetrick, 1982). The purpose of the present report is to provide a user's manual for the computer code, TOX-SCREEN, which implements the multimedia model.

The computer code (machine readable program) for TOX-SCREEN is available from the Office of Toxic Substances, Exposure Evaluation Division, where the master code is maintained and where all changes to the program are documented. User support is also provided by the Office of Toxic Substances.

The TOX-SCREEN computer code is written in the FORTRAN language. The program has separate modules and related subroutines for calculating results in the air, water, and soil media, yet allows intermedia transport of chemicals. Likewise, separate input data files are needed for each media. That is, the code is not interactive in that it does not prompt the user for information during execution, but reads all the data from input files. Once the input data are compiled, the TOX-SCREEN program can be run with ease by executing it directly from a computer terminal or by submitting it with the proper job control language (JCL) to a computer.

Before describing the subroutine structure and individual modules of TOX-SCREEN in detail (Section 3), a brief description of the model assumptions and structure is given in this document (Section 2). In Section 4, details concerning the mode of operation of the code, the input sequence, and input format are provided, followed by a description of code output in Section 5. A discussion summarizing the information in this report is then provided in Section 6. Appendix A of this report provides a table of input parameters and other important parameters that are used

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frequently in the program and their definitions, to allow the user quick access to this information. A listing of the JCL needed to submit TOXSCREEN for execution on the ORNL IBM 3033 computer is given in Appendix B.

2. MODEL DESCRIPTION

Because TOX-SCREEN is proposed as a screening tool for evaluating chemicals with respect to their human exposure potential, the model is simplified to minimize user input requirements and is overpredictive (conservative) in nature for many aspects of chemical transport. To facilitate use of the model for a large number of assessments in a relatively short period of time, a number of simplifying approaches to model development were adopted. First, in order to minimize data collection for users, a generic approach to simulating pollutant transport in the environment was taken. The model assumes a generic positioning of surface water bodies relative to atmospheric pollutant sources and contaminated land areas. It also makes use of data that are typical of large geographic regions or of the entire United States, rather than site-specific data. Second, equations used in TOX-SCREEN were selected to achieve a balance between simplicity and flexibility believed to be necessary to fulfill user needs. Conservatism is achieved to varying degrees depending on generic values assigned to various parameters but is ensured to some extent by model structure.

The multimedia nature of TOX-SCREEN requires that physical/chemical processes which drive transport of chemicals across air-water, air-soil, and soil-water interfaces be simulated. Such media interactions are handled explicitly in the model in most cases, with the use of deposition velocities, transfer rate coefficients, and mass loading parameters. Monthly pollutant concentrations in air, surface water, and soil reflect both direct input to any or all of the media from a specified source(s) and subsequent interaction via processes such as volatilization, atmospheric deposition, and surface runoff. The user must select the types of water bodies (i.e., river, lake, estuary, or ocean), if any, to be considered in any given simulation, as well as specify whether the pollutant is directly released to air or water and/or directly applied to soil. A brief discussion of methods employed to simulate atmospheric and aquatic dispersion of chemicals, their dispersion in soil, and intermedia transport in TOX-SCREEN is provided below. More detail, and the equations pertinent to these topics, are given in McDowell-Boyer and Hetrick (1982) and Appendix F of the present report.

2.1 ATMOSPHERIC DISPERSION

2.1.1 Point Sources

A modification of the original Gaussian plume equation of Pasquill (1961) is adapted in TOX-SCREEN for use in estimating downwind concentrations of a particular chemical emitted from a point source. Modifications to the basic equation were made such that the TOX-SCREEN model considers plume depletion due to wet and dry deposition processes, gravitational settling, and chemical degradation. Also, provisions were made to allow calculation of sector-averaged concentrations for predetermined sector width and user-specified sector length, as well as the downwind maximum centerline concentration.

Sector-averaged and maximum ground-level atmospheric concentrations are calculated on a monthly average basis, assuming a constant Pasquill Stability Category D (i.e., neutral conditions). Although this assumption would not necessarily constitute worst-case conditions, the additional assumption that the wind direction is constant throughout the model application time period, in the direction of maximum concentration, does incorporate conservatism into the overall calculation.

2.1.2 Area Sources

A simple urban diffusion model (Gifford and Hanna, 1973; Hanna, 1977) has been adopted for use in estimating ground-level pollutant concentrations over area sources. Concentrations are calculated as a function of stability (again assumed to be neutral), area size, source strength and wind speed. Chemical degradation is handled by applying a first-order exponential term to the calculated concentration. Depletion of the air concentration due to deposition is not handled in the area source model. Indications are that consideration of deposition will not significantly affect the calculated concentrations in light of uncertainties associated with the model predictions (McDowell-Boyer and Hetrick, 1982).

2.2 AQUATIC DISPERSION

2.2.1 Rivers

For dispersion in rivers, the user must select the number and size of reaches to be simulated, with the restriction that each must be considered geometrically equivalent (i.e., same length, width, and depth) and have the same flow rate. The purpose of breaking the river up into reaches is thus to allow estimation of concentration at various points downstream of a source term.

An equation similar to the USEPA EXAMS model equation (Smith et al., 1977; Burns et al., 1982) is used to estimate the monthly pollutant mass in each reach. The equation is based on the assumption of complete and instantaneous mixing in each reach upon introduction of a pollutant.

Monthly pollutant concentrations are calculated by dividing the pollutant mass by the reach volume. The concentrations are reported as dissolved neutral, dissolved ionic, and adsorbed forms, in accordance with chemical equilibria considerations. To estimate adsorption onto sediment, the concentration of the suspended sediment is either required as input or estimated according to Laursen′s formula (Laursen, 1958).

2.2.2 Lakes

The same mass balance equation used for rivers (i.e., the EXAMS approach) is applied to lakes in TOX-SCREEN, again necessitating the assumption of complete and instantaneous mixing. Concentrations are calculated for the dissolved neutral, dissolved ionic, and adsorbed forms based on lake volume and chemical equilibria. Suspended sediment concentrations in lakes are required as input, when at all possible. In lieu of appropriate data, however, a means of estimating a lake sediment concentration from the suspended sediment concentration in a tributary is provided.

2.2.3 Estuaries

A one-dimensional steady-state model that assumes constant cross-sectional area (A), a constant tidally and sectionally averaged longitudinal dispersion coefficient (E_L), and a constant fresh water velocity (v_f) is used for simulating dispersion of pollutants in estuaries. The model is documented as acceptable to predict radionuclide transport for releases of long duration (i.e., long with respect to time to achieve steady state) in the U.S. Nuclear Regulatory Commission's (USNRC) Regulatory Guide 1.113 (USNRC, 1977).

Pollutant concentrations of the dissolved neutral, dissolved ionic, and adsorbed forms are again computed. The estuary is broken up into "reaches" representing variable distances up- and downstream of the source in order to observe concentration gradients. Suspended sediment concentrations in estuaries must be input by the user.

2.2.4 Oceans

A steady-state Gaussian-type linear diffusion model is used to estimate dispersion of pollutants potentially discharged to ocean coastal waters (Brooks, 1960). Models of this type are recommended in the USNRC Regulatory Guide 1.113 (USNRC, 1977) when detailed descriptions of the field of predicted concentrations are not required. The ocean dispersion model chosen is that described by Brooks (1960) for diffusion of sewage effluents. Critical assumptions include offshore discharge via an outfall terminating in a multiple-point diffuser, movement of the resulting pollutant field at the same rate as the prevailing current, negligible vertical and longitudinal mixing and steady flow.

The centerline concentration on the ocean shelf will, of course, decrease as a function of distance out from the diffuser. The user may choose any number of distances to calculate concentration. Pollutant concentrations of dissolved neutral, dissolved ionic, and adsorbed forms are output. Suspended sediment concentrations for ocean shelves must be input by the user.

2.3 DISPERSION IN SOIL

At the request of EPA, the TOX-SCREEN model employs the Arthur D. Little (ADL) SESOIL model (Bonazountas and Wagner, 1981) to estimate concentrations of a pollutant in the soil media following introduction via direct application and/or interaction with other media (i.e., deposition from air). In this model, simulated hydrologic processes, volatilization, and erosion by wind all serve to transport the pollutant from its point of introduction (i.e., to the upper, middle, or lower region of a soil column) through the column to other media. The SESOIL model is statistical and seasonal, with respect to the hydrologic cycle, and provides estimates of pollutant distributions within the soil column on an annual or monthly basis, although a provision is reportedly made for storm-by-storm simulations (Bonazountas and Wagner, 1981). At present, the SESOIL model does not address pollutant movement in saturated groundwater.

Output of the SESOIL model includes pollutant concentrations in the soil water (μg/ml), soil air (μg/ml), and adsorbed phases (μg/g) in both the upper, middle, and lower unsaturated soil zones. The amount of pollutant lost from the unsaturated soil zones per unit area (cm^2) is provided in terms of μg lost via surface runoff, percolation to groundwater, volatilization, biodegradation, chemical degradation, surface washload (erosion by water) and resuspension (erosion by wind). Final equations describing the latter two processes have not been provided in SESOIL to date, but empirical equations or values for soil erosion (washload) and dust loading (resuspension) per unit area are used in TOX-SCREEN until such equations are in place (see McDowell-Boyer and Hetrick, 1982).

2.4 INTERMEDIA TRANSPORT

Processes which serve to transport chemicals across media interfaces include deposition of airborne pollutants onto water and soil surfaces, volatilization of chemicals from these surfaces, surface and groundwater runoff, and soil erosion via water or wind. Deposition is a result of both dry and wet processes, and is handled in TOX-SCREEN via dry deposition velocities and washout ratios, respectively.

Volatilization from surface water bodies is estimated in TOX-SCREEN with a user-supplied volatilization rate constant. A means of estimating such a rate constant in lieu of empirical data is provided in McDowell-Boyer and Hetrick (1982). Volatilization from soil is simulated within the SESOIL code, as is surface and groundwater runoff (the latter term implying transport into the saturated zone). The net groundwater runoff is assumed to recharge the adjacent surface water inventory immediately and completely, because no groundwater storage or retardation of movement is presently modeled in SESOIL.

Soil erosion may result in transport of chemicals adsorbed to surface soil, and is handled in TOX-SCREEN with an empirically derived equation based on annual precipitation (McDowell-Boyer and Hetrick, 1982). Resuspension may result in enhanced air concentrations of adsorbed chemicals, and is simulated in TOX-SCREEN with the use of empirical dust loading values.

In order for the simulation of processes described above to result in a quantitative assessment of intermedia transport, the relative locations of the media as well as the size of the contaminated area must be designated. Such designations are detailed in McDowell-Boyer and Hetrick (1982). Briefly, if a water body or soil is contaminated from deposition of a plume (i.e., due to a point source), the contamination area is delineated in TOX-SCREEN by the shape of the plume which has intercepted the ground and/or water surface. If contamination occurs from deposition of a pollutant from an area source, the area(s) of the water body(ies) is (are) specified by the user and is (are) assumed to be within the total area.

The location of the contaminated water body or land area relative to an atmospheric point source is always assumed to encompass the point of maximum downwind concentration. The approach taken for an area source dictates a uniform deposition throughout the area specified, such that the location of the water body within that area is unimportant. However, contaminated soil areas are always assumed to be adjacent to water bodies present to maximize subsequent water contamination, whether the initial contaminating event is due to an atmospheric source or direct application to the soil.

Whenever a water body (except on coastal waters) is contaminated, the volatilization process is assumed to contaminate the air directly above the water body, which is treated as an area source. Likewise, the air above a contaminated soil area (treated as an area source) is contaminated via volatilization or resuspension processes.

Media interactions between coastal waters and air or soil, and interactions between water bodies are not presently considered in TOX-SCREEN. Therefore, concentrations in oceans reflect only contamination via direct input from offshore discharge. Furthermore, interactions between surface or ground water and soil ignore contamination of soil via irrigation with polluted waters. It may be possible for the TOX-SCREEN user to consider this latter interaction by determining a direct application rate for input to the SESOIL module based on knowledge of the amount of water used in irrigation as well as on the pollutant concentration in that water.

2.5 BIOACCUMULATION

Methods adopted to estimate bioaccumulation of chemicals in aquatic organisms, terrestrial food animals, and plants are described in detail in Appendix F. Briefly, bioaccumulation in aquatic organisms is estimated via a bioaccumulation factor [BCF(aq)], which is defined as the ratio between a compound's concentration in an organism to its concentration in the surrounding water. The bioaccumulation factor is estimated from an empirically determined relationship between BCF(aq) and the octanol-water partition coefficient, K_{ow}. A number of limitations are associated with this method and are discussed in Appendix F.

Bioaccumulation in terrestrial food animals such as beef cattle is handled in TOX-SCREEN in a more crude manner due to a poorer correlation between BCF and K_{ow} than exists for aquatic organisms. A single numerical value of log K_{ow} is used to screen chemicals with respect to their bioaccumulation potential. Again, limitations imposed by this method are outlined in Appendix F.

Bioaccumulation in terrestrial plants is estimated in TOX-SCREEN in two distinct steps: one step is to estimate vegetation concentrations due to root uptake and another step to estimate concentrations due to direct interception of depositing chemicals from the air. The root uptake estimation relies on an empirical relationship between BCF (plants) and the soil-water partition coefficient (K_d). The K_d is estimated from the organic carbon sorption coefficient and the percent organic carbon, both of which are required input to the SESOIL portion of TOX-SCREFN. The estimation of bioaccumulation due to interception in TOX-SCREEN is estimated using a model developed by Chamberlain (1970). The concentration due to interception is estimated as a function of an empirically determined initial interception fraction, the vegetative productivity, an empirical weathering constant, the crop growth period before harvest, and the deposition rate. The total concentration in vegetation is then determined in TOX-SCREEN by summing the concentrations due to root uptake and interception.

3. STRUCTURE OF THE TOX-SCREEN PROGRAM

This section presents the overall structure of the TOX-SCREEN computer code and summarizes the user options available in the model. A discussion of how the SESOIL program (Bonazountas and Wagner, 1981) was adapted for use in TOX-SCREEN is also given. Descriptions of the TOX-SCREEN subroutines follow. The listing of the program can be found in Appendix E.

3.1 SUBROUTINE STRUCTURE

TOX-SCREEN consists of 27 routines in all, 15 of which have been adapted for use from the SESOIL model (Bonazountas and Wagner, 1981). The remaining 12 routines are called READIN, SEDCON, FUNLAU, SPLEVA, ALPHA, AIR, DEPAVG, CAVGE, WATER, BIOCHN, OUTPUT and D01AJF, the latter being a general-purpose integrator package (NAGFLIB, 1981). The SESOIL routines used are called MAIN (main program), RFILE, LEVEL3, HYDROM, HYDROA, WATCON, FGAMA, GAMA, FIE, FII, LINT, TRANS3, VOLM, DEPTH, and COMP. The above subroutines are named according to their functions, and various COMMON statements and parameter names within the routines are named in such a way as to be recognized by the user. Figure 1 shows the structure and gives brief descriptions for the routines of the model. The subroutine BIOCHN has been added most recently, and the equations coded in this routine are documented in Appendix F of this report.

As shown in Fig. 1, the MAIN program calls routines RFILE and READIN to read the input data. MAIN then calls LEVEL3 which coordinates all activities between the SESOIL routines adapted for the model and the rest of the TOX-SCREEN subprograms. LEVEL3 first calls subroutine HYDROM which collaborates with other SESOIL subprograms (see Fig. 1) to compute the hydrological parameters (soil moisture, precipitation, infiltration, evapotranspiration, surface runoff, and groundwater runoff). Next, if a water body is considered and if sediment concentrations have not been input by the user, LEVEL3 can call SEDCON, which in turn calls FUNLAU and SPLEVA, to compute them. Then ALPHA is called by LEVEL3 to compute the ionization fractions. Up to this point, the program has computed parameters needed

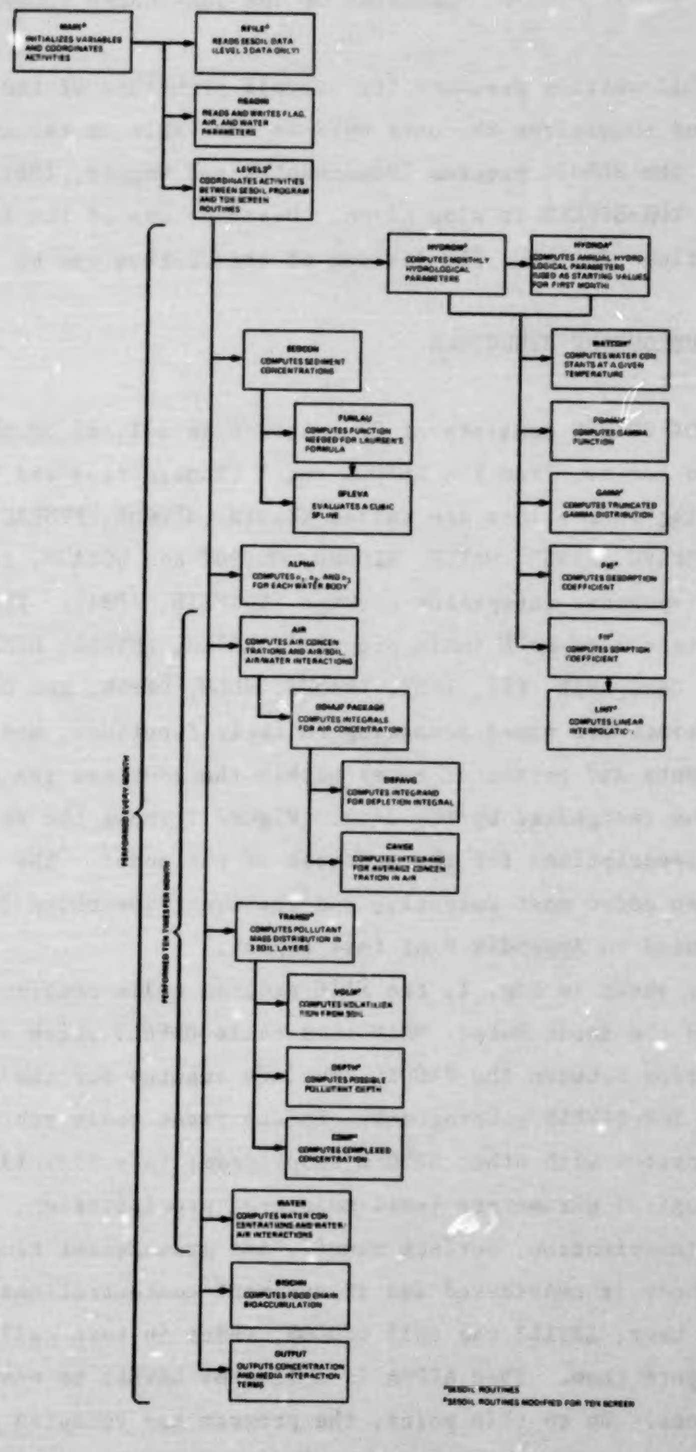
ORNL-DWG 82-19445
MAIN
INITIALIZES VARIABLES AND COORDINATES ACTIVITIES
RFILE
READS SESOIL DATA (LEVEL 3 DATA ONLY)
READIN
READS AND WRITES FLAG, AIR, AND WATER PARAMETERS
LEVELS
COORDINATES ACTIVITIES BETWEEN SESOIL PROGRAM AND TOX SCREEN ROUTINES
HYDROM
COMPUTES MONTHLY HYDROLOGICAL PARAMETERS
HYDROA
COMPUTES ANNUAL HYDROLOGICAL PARAMETERS (USED AS STARTING VALUES FOR FIRST MONTH)
SEDCON
COMPUTES SEDIMENT CONCENTRATIONS
FUNLAU
COMPUTES FUNCTION NEEDED FOR LAURSEN'S FORMULA
SPLEVA
EVALUATES A CUBIC SPLINE
ALPHA
COMPUTES α_1, α_2, AND α_3 FOR EACH WATER BODY
AIR
COMPUTES AIR CONCENTRATIONS AND AIR/SOIL, AIR/WATER INTERACTIONS
QDHAJF PACKAGE
COMPUTES INTEGRALS FOR AIR CONCENTRATION
DEPAVG
COMPUTES INTEGRAND FOR DEPLETION INTEGRAL
CAVGE
COMPUTES INTEGRAND FOR AVERAGE CONCENTRATION IN AIR
TRANS2
COMPUTES POLLUTANT MASS DISTRIBUTION IN 3 SOIL LAYERS
VOLM
COMPUTES VOLATILIZATION FROM SOIL
DEPTH
COMPUTES POSSIBLE POLLUTANT DEPTH
COMP
COMPUTES COMPLEXED CONCENTRATION
WATER
COMPUTES WATER CONCENTRATIONS AND WATER/AIR INTERACTIONS
BIOCHN
COMPUTES FOOD CHAIN BIOACCUMULATION
OUTPUT
OUTPUTS CONCENTRATION AND MEDIA INTERACTION TERMS
WATCON
COMPUTES WATER CONSTANTS AT A GIVEN TEMPERATURE
FGAMA
COMPUTES GAMMA FUNCTION
GAMA
COMPUTES TRUNCATED GAMMA DISTRIBUTION
FKE
COMPUTES DESORPTION COEFFICIENT
FKI
COMPUTES SORPTION COEFFICIENT
LINT
COMPUTES LINEAR INTERPOLATION
PERFORMED EVERY MONTH
PERFORMED TEN TIMES PER MONTH
aSESOIL ROUTINES
bSESOIL ROUTINES MODIFIED FOR TOX SCREEN

Figure 1. Structure of the TOX-SCREEN Program

later in solving the major equations of the model. LEVEL3 then calls the three major routines AIR, TRANS3, and WATER to compute pollutant concentrations in the air, soil, and water, respectively. Media interactions in the model are passed from one subroutine to another in a major "DO loop". Next, LEVEL3 calls BIOCHN which computes the food chain bioaccumulation. Finally, LEVEL3 calls OUTPUT to write out the results.

The pollutant cycle equations are formulated on a monthly basis. However, since all terms with a time-dependent expression in the TOX-SCREEN model are written with an explicit time step (e.g., see eq. 3-1 in McDowell-Boyer and Hetrick (1982) and Table PT-5 in Bonazountas and Wagner (1981)), time steps smaller than one month are used to increase accuracy in solving these expressions. Inspection of Fig. 1 shows that the hydrologic processes, the sediment concentrations (in water), the ionization fractions, and the food chain concentrations are computed only once a month, in that equilibrium expressions describe the underlying processes in the model. All other equations in the model are solved using smaller time steps (presently 10 steps per month). All input parameters to the model are either constant or monthly values (see Section 4). The output of the model contains end-of-the-month values of pollutant concentrations for each media; the monthly results output for intermedia transport processes (e.g. deposition, volatilization, etc.) represent the summation of results of the smaller time steps. More details of the output are given in Section 5.

3.2 USER OPTIONS

Fig. 1 shows how the routines are connected to each other, but does not show the numerous options available to the user in running the TOX-SCREEN code. Although a thorough discussion of these options is given in Section 4, a brief summary is given now to assist the reader while reading the subroutine descriptions given below. TOX-SCREEN is structured to be able to run up to four separate simulations simultaneously, with a different water body type (lake, river, estuary, ocean) used for each simulation. That is, given the same air and soil parameters, a separate simulation is necessary to compute results for each water body type specified. A separate run can be made where no water bodies are considered, in which case, TOX-SCREEN considers interactions between soil and air only. The user has the option of picking either an area or point source for the air compartment or specifying that there be no air source at all. If there is an air source, the pollutant must be specified to be either a particulate or gas. Pollutant sources can be input to all three media (air, water, soil) simultaneously, or to one or any combination of the three. If a water body is being considered (or water bodies), the chemical must be specified as acidic, basic, or neither. Rate constants for hydrolysis, oxidation, and volatilization and the value of the soil-water partition coefficient must be specified for each water body due to their potential dependence on pH and/or water velocity (Browman, Patterson, and Sworski, 1982; Browman and Chesters, 1977). For lakes and rivers, sediment concentrations can be either input directly, or computed using given input parameters. Sediment concentrations for estuaries or oceans must be input directly. For estuaries, the longitudinal dispersion coefficient can be input directly, or if unknown, can be computed using given input data. For the bioaccumulation subroutine (BIOCHN), the user must specify whether the compound is or is not a covalently bonding material.

3.3 ADAPTATION OF THE SESOIL MODULE

The statistical and seasonal SESOIL model has been adapted for TOX-SCREEN to estimate concentrations of pollutant in the soil following direct pollutant application and/or interaction with the air compartment. SESOIL interacts with other media through simulated hydrological processes, volatilization, and resuspension by wind. All processes in the SESOIL model have been documented by Bonazountas and Wagner (1981). The following describes briefly the modifications made to SESOIL in adapting it for TOX-SCREEN.

Although SESOIL is designed to operate at four different levels (LEVEL0, LEVEL1, LEVEL2, and LEVEL3 - see Bonazountas and Wagner, 1981), only the LEVEL3 portion of the model was adapted for use in TOX-SCREEN.

Because of time resolution requirements, the LEVEL0 and LEVEL1 modes of operation (annual simulations) could not be considered for use in the TOX-SCREEN model. LEVEL2 and LEVEL3 both perform operations monthly, but LEVEL3 is more flexible with respect to applications in that it considers three unsaturated soil layers instead of just two by LEVEL2. Thus, LEVEL3 was adapted for use by TOX-SCREEN.

Some of the routines in SESOIL were not needed for the LEVEL3 mode of operation and thus were not adapted. Figure 1 shows the SESOIL routines that are in TOX-SCREEN and, in particular, shows those SESOIL routines that were modified for use in TOX-SCREEN. Although care was taken to change these routines as little as possible (to allow for future updates by the authors of SESOIL, and so as not to alter the calculational steps in the program), some changes were necessary in order to adapt the routines in TOX-SCREEN. Detailed descriptions of the SESOIL routines will not be given here since they have been documented by Bonazountas and Wagner (1981). However, the following discussion addresses the changes to those routines that were modified.

3.3.1 Changes to SESOIL Subroutine MAIN

The MAIN program of SESOIL was modified to become the MAIN program for TOX-SCREEN. A number of parameters needed for TOX-SCREEN were initialized to 0.0 and passed to the other routines via COMMON statements. MAIN is no longer capable of calling subroutines LEVEL0, LEVEL1, or LEVEL2 since these routines were removed. Subroutine RFILE is still called from MAIN as in the SESOIL code. A call to subroutine READIN was inserted. All other additions and changes to this routine were minor.

3.3.2 Changes to SESOIL Subroutine RFILE

Portions of subroutine RFILE concerning the reading of data for LEVEL0, LEVEL1, and LEVEL2 were removed. Thus, RFILE will now read data for only the LEVEL3 mode of operation, although it is still capable of reading any existing SESOIL data files (Bonazountas and Wagner, 1981).

RFILE will skip over any LEVEL0, LEVEL1, or LEVEL2 data in the data files until it reaches the appropriate LEVEL3 data. More information is given in Section 4 where the input data for the SESOIL portion of TOX-SCREEN is thoroughly explained.

3.3.3 Changes to SESOIL Subroutine LEVEL3

LEVEL3 is the main connecting link between the adopted SESOIL routines and the other routines of the TOX-SCREEN model. One of the major changes made was to put the monthly "DO loop" *around* the calls to subroutines HYDROM and TRANS3, and the monthly "DO loop" *within* HYDROM and TRANS3 were removed. Also, the "DO LOOP" for the number of steps per month was removed *within* TRANS3 and put *around* the call to TRANS3 in subroutine LEVEL3. These changes allowed the interactions between HYDROM and TRANS3 and the routines SEDCON, ALPHA, AIR, WATER, and OUTPUT, as specified by the TOX-SCREEN structure (see Fig. 1). For any one time step, LEVEL3 now determines for what water body types the user desires results and keeps track of these results separately (see discussion of TRANS3 below). A call to subroutine OUTPUT was inserted at the end of LEVEL3 in order for monthly results to be written into output files.

3.3.4 Changes to SESOIL Subroutine HYDROM

The only major change in HYDROM was the removal of the monthly "DO loop" from *within* the routine and putting it *outside* the call to HYDROM in the LEVEL3 subroutine. Thus, the monthly index (computer name IMO) is now passed through the argument list of HYDROM so that calculations within the routine are done for each month. Constants calculated within HYDROM are computed only during the first step (IMO=1) to avoid repetition.

3.3.5 Changes to SESOIL Subroutine TRANS3

Both the monthly and the number of steps per month "DO loops" were removed from *within* TRANS3 and put *outside* the call to this routine in subprogram LEVEL3. The monthly index (IMO) and the steps per month index (ISTEP) are now passed through the argument list of TRANS3 so that computations within TRANS3 are done for each step. Also, media interaction terms (e.g., deposition from air to soil, pollutant transport from soil to water, and volatilization from soil to air) are passed through the argument list. In particular, deposition from air to soil is computed in subroutine AIR, passed via COMMON statement to subprogram LEVEL3, and then passed through the argument list to TRANS3 for each time step. These terms are kept track of separately in LEVEL3 for each water body considered. The pollutant concentrations computed in TRANS3 for three soil layers are also passed through the argument list and stored separately in LEVEL3 for each water body specified by the user. For example, if both a lake and river were considered in a particular computer run, then for each time step LEVEL3 calls TRANS3 twice, once passing parameters computed for the lake case and once passing parameters computed for the river case. For each water body, TRANS3 computes the adjacent soil concentrations and passes these values back to LEVEL3 where they are stored. At the beginning of the next time step, these concentrations are passed back to TRANS3 and used in further calculations.

In the SESOIL code, TRANS3 also outputs results in a separate file. This capability was kept for TOX-SCREEN but a few coding changes were needed and some additions were made. This output is discussed further in Section 5.

It is noted here that the call to subroutine TRANS3 is bypassed in LEVEL3 for ocean simulations. Media interaction between coastal waters and soil is not presently considered in TOX-SCREEN.

3.4 TOX-SCREEN SUBPROGRAM DESCRIPTIONS

Discussion of each of the TOX-SCREEN subroutines, other than SESOIL routines, are given below. If the user desires more details about the code, Appendix A provides an alphabetical list and description of important parameters in the code which should be useful.

3.4.1 Subroutine READIN

Subroutine READIN reads the input data, other than that for SESOIL, for TOX-SCREEN. Separate input files are needed for model flags, air parameters, and water parameters. This input is discussed thoroughly in Section 4. After reading the data, READIN outputs the data into a file in tabular form. This helps the user determine whether the data were input correctly. Where appropriate, various warning messages are written into this file if the program can recognize that the data are not logical. This output file is discussed further in Section 5.

3.4.2 Subroutine SEDCON

Subroutine SEDCON is an optional routine that can be used to compute sediment concentrations for lakes or rivers if these values are unknown. The descriptions of the model flags in Section 4 explain what these options are in detail. Basically, if the sediment concentration in a lake under consideration is unknown, but the sediment concentration of a tributary flowing into the lake is known, SEDCON will use this information to estimate the lake sediment concentration (see McDowell-Boyer and Hetrick, 1982). The trapping efficiency of the lake P_t is needed in this calculation and is computed in SEDCON by use of a cubic spline that was fit to a curve given in Zison et al. (1977). The coefficients of the cubic spline were computed separately and appear in DATA statements in SEDCON. FUNCTION SPLEVA (see below) is used to evaluate the spline. Thus, the user does not have to provide this parameter. If the tributary sediment concentration is unknown, but values are known for the median sediment diameter, sediment density, water density, depth, and slope of the tributary, then SEDCON will call FUNLAU (see below) to assist in computing the sediment concentration of the tributary using Laursen's formula (Laursen, 1958). Likewise, this last statement applies to rivers or streams as well.

3.4.3 Subroutine FUNLAU

This subprogram is used to compute Laursen's function and other parameters needed for computing sediment concentration in water by Laursen's formula (Laursen, 1958; also, see McDowell-Boyer and Hetrick, 1982). First, FUNLAU computes the Shields factor ϕ by use of a cubic spline that was fit to the curve given in Bagnold (1966). The sediment fall velocity w is needed for Laursen's function and is computed by use of a cubic spline that was fit to a curve given in Fields (1976). The only input parameter needed in computing both ϕ and w is the median sediment particle diameter d. The coefficients of the cubic splines were computed separately for each curve and appear in DATA statements in FUNLAU. Thus, FUNLAU passes d and the appropriate coefficients to FUNCTION SPLEVA (see below) and ϕ is computed; likewise, the same is done in computing w. The critical tractive force (needed for Laursen's formula) is computed using ϕ, the water density, the sediment density, and d. The independent variable needed for Laursen's function is computed using w, the acceleration of gravity, and the input parameters for water depth and river slope (see McDowell-Boyer and Hetrick, 1982). Finally, Laursen's function is computed by use of a cubic spline that was fit to the curve given by Laursen (1958). These computations are passed back to subroutine SEDCON, where the sediment concentration is then computed.

3.4.4 Function SPLEVA

The sole purpose of SPLEVA is to evaluate a cubic spline function by using Horner's rule (Forsythe, et al., 1977). SPLEVA is used by both subroutine SEDCON and FUNLAU.

3.4.5 Subroutine ALPHA

Subroutine ALPHA computes the ionization fractions α_1, α_2, and α_3 which are used in computing water pollutant concentrations in dissolved neutral, dissolved ionic, and adsorbed forms, respectively (see McDowell-Boyer and Hetrick, 1982). Since the sediment concentration and the concentration of H^+ are needed in computing the α's, and since these values can be different for each water body type (i.e., lake, river, estuary, ocean), ALPHA computes and stores the α's separately for each water body type considered. If the user wants only soil and air interaction for a particular simulation (i.e., no water body is considered), then subroutine ALPHA is bypassed.

3.4.6 Subroutine AIR

Subroutine AIR is one of the major routines of the TOX-SCREEN model. It computes the maximum and average air pollutant concentrations as well as the pollutant deposition rates to soil and water for each water body that is being considered. The first thing that AIR does is determine what kind of pollutant source there is to the air compartment (point source, area source, or none). If there is no point or area source (i.e., none is specified), subprogram AIR still needs to compute concentrations in the air due to volatilization from the soil and water compartments. An area source box model is used for these calculations (see McDowell-Boyer and Hetrick, 1982). AIR does these calculations separately for each water body that is being considered in the simulation. Deposition rates back to the soil and water compartments are computed also. TOX-SCREEN assumes that if the pollutant volatilizes to the air, it will be in a gaseous form. Thus, the deposition rates for redepositing volatilized material are calculated using wet and dry deposition velocities for gases. AIR is capable of handling the case when no water body is considered; i.e., only soil and air interactions are simulated.

When a point source is specified, subprogram AIR first computes the effective stack height due to plume rise (see McDowell-Boyer and Hetrick 1982). The maximum ground-level concentration χ_{max} is then computed. The general-purpose integrator package D01AJF (see below) is called to aid in computing the depleted source term Q_p, which is needed in calculating χ_{max} (McDowell-Boyer and Hetrick, 1982). Then, for each water body under consideration, subroutine AIR computes the average concentrations and wet and dry depositions due to the point source. Again, the D01AJF package is called to compute the necessary integrations. Added to these results are computations due to volatilization rates to the air from the soil and water compartments. If no water body is being considered, then AIR considers interaction between soil and air only.

The computations are much simpler if an area source is specified by the user. No integrations are necessary as a simple urban diffusion box model is used (see McDowell-Boyer and Hetrick, 1982). Only one average air concentration is computed per month in this case, and this calculation considers the area source strength that is input by the user and the calculated source strength due to volatilization from the soil and water. TOX-SCREEN assumes that each water body specified is within the area source. If no water body is specified, then only interactions between the air and soil are considered.

The maximum and average air concentrations and the deposition rates to the soil and water compartments are passed from AIR to the appropriate TOX-SCREEN routines via COMMON statements. Likewise, volatilization rates from the soil or water compartments come to AIR through COMMON statements. All other parameters needed for this routine are either passed through the argument list of AIR or are in COMMON.

3.4.7 The D01AJF Package

The D01AJF package consists of the subroutine D01AJF and auxiliary routines D01AJV, D01AJX, D01AJY, D01AJZ, P01AAF, P01AAZ, X02AAF, X02ABF, X02ACF, and X04AAF. D01AJF is from the NAG FORTRAN library (NAGFLIB, 1981) and is a general-purpose integrator which calculates an approximation to the integral of a function over a finite interval. Subroutine AIR calls the D01AJF package when a point source is specified to compute the integrals used in the point source equations (McDowell-Boyer and Hetrick, 1982). D01AJF calls function routines DEPAVG and CAVGE which supply the integrands needed (see below). Three machine-dependent numbers appear in the D01AJF package. The REAL FUNCTION X02AAF should be set to ε where, ε is the smallest number on the computer such that $1.0+\varepsilon>1.0$. The REAL FUNCTION X02ABF is the smallest positive real floating-point number representable on the computer and REAL FUNCTION X02ACF is the largest real floating-point number representable on the computer. Since D01AJF has been fully documented, no further discussion will be included here.

3.4.8 Function DEPAVG

Function DEPAVG computes the integrand of the integral needed to deplete the source strength from a point source (McDowell-Boyer and Hetrick, 1982). DEPAVG is called from the D01AJF package.

3.4.9 Function CAVGE

Function CAVGE computes the integrand of the integral needed for the sector-averaged concentration in air due to a point source (McDowell-Boyer and Hetrick, 1982). CAVGE is called from the D01AJF package.

3.4.10 Subroutine WATER

This subprogram computes the pollutant concentrations in the water and the volatilization rates from the water to the air for each water body specified by the user. For lakes, rivers, and estuaries, subroutine WATER can accept direct pollutant input (e.g., from a plant) as well as pollutant rates from both the soil and air compartments. For oceans, only direct source input by the user is accepted since TOX-SCREEN does not consider media interaction for oceans. The water concentrations are calculated in the dissolved neutral, dissolved ionic, and adsorbed forms by using the coefficients computed in subroutine ALPHA. These concentrations are stored separately for each water body type considered. The equations coded in subroutine WATER are documented by McDowell-Boyer and Hetrick (1982).

3.4.11 Subroutine BIOCHN

BIOCHN has been added recently to the TOX-SCREEN model to estimate bioaccumulation in food chains. The methods used for these estimations are documented in Appendix F of this report. Since BIOCHN is a recent addition to the computer code, and time did not permit assimilation into the overall code framework, the input data needed for the BIOCHN equations are read by BIOCHN itself from a separate input data file. Also, all results from BIOCHN are written by BIOCHN into a separate computer file. The input data for and the output from BIOCHN are discussed further in Sections 4 and 5, respectively.

Basically, BIOCHN reads the necessary input data and immediately writes these data into a file in tabular form so that the user can determine if they were input correctly. Other parameters needed in the bioaccumulation equations are passed to BIOCHN via COMMON statements. Then, for each water body type specified, BIOCHN computes concentrations in aquatic organisms and terrestrial plants. For each month, the maximum pollutant concentration in each water body (computed by subroutine WATER) is used in computing the concentration in the aquatic organisms. The monthly results are printed in tabular form into an output file (see Section 5).

3.4.12 Subroutine OUTPUT

The sole purpose of subroutine OUTPUT is to write out results from the TOX-SCREEN calculations. A separate output file is written for each water body that is specified by the user. For example, if a lake was specified, the monthly pollutant concentrations for the water in the lake, the soil next to the lake, and the air above the lake and soil, as well as the monthly interaction terms (deposition, volatilization, etc.) would be printed in an output file. If a river was specified during this same computer run, a different file would include the results for the river. More details are given about the output from subroutine OUTPUT in Sections 4 and 5.

4. TOX-SCREEN OPERATION

This section presents to the user the necessary information on how to run the TOX-SCREEN computer code. A complete discussion of input data compilation is included. While reading this section, it will be helpful to refer to Appendixes B and C, which contain the job control language (JCL) to run TOX-SCREEN on the ORNL IBM 3033 computer and sample input data, respectively.

4.1 MODE OF OPERATION

Before execution of TOX-SCREEN is possible, the user must first assemble seven input data files. The program reads these data files by use of seven different logical input device numbers. Table 1 shows the logical input device numbers that are used in TOX-SCREEN and gives a short description of the files corresponding to these device numbers. It is important for the user to assign the proper device number to the correct file. For example, the logical device number 10 is used to read the file that contains the model flags. On the local ORNL PDP-10 computer, this file could be named FOR10.DAT. Similarly, the other files could be named FOR01.DAT, FOR02.DAT, FOR05.DAT, FOR11.DAT, FOR12.DAT, and FOR18.DAT. These input data files are discussed in the following subsections. To execute TOX-SCREEN on the ORNL PDP-10 computer, the user simply types into the terminal:

```
ASSIGN DSK 5↓
ASSIGN DSK 6↓
EX SCREEN.TOX, SYS:ERF.REL↓
```

Here, the symbol ↓ stands for carriage return. The user types the first two lines since device numbers 5 and 6 are default numbers for the teletype for input and output, respectively, on the ORNL PDP-10 computer. Since TOX-SCREEN reads data from a file with device number 5 (FOR05.DAT) and outputs results into another file with device number 6 (FOR06.DAT), these numbers must be assigned first before executing the program on the PDP-10. For example, if the user did not assign the number 6, then the results from the

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Table 1. Logical Input Device Numbers in TOX-SCREEN

Device Number	ORNL PDP-10 Data File	Data Description
5	FOR05.DAT	SESOIL data file containing executive data (Bonazountas and Wagner, 1981).
1	FOR01.DAT	SESOIL data file containing general climatologic, soil, and chemistry data.
2	FOR02.DAT	SESOIL data file containing data for LEVEL3 executions.
10	FOR10.DAT	Data file containing the model flag parameters.
11	FOR11.DAT	Data file containing the air compartment parameters.
12	FOR12.DAT	Data file containing the water compartment parameters.
18	FOR18.DAT	Data file containing the bioaccumulation parameters.

TOX-SCREEN program using unit 6 would be typed into an arbitrarily named file during execution on the PDP-10 rather than be typed into file FOR06.DAT. On the third line above, SCREEN.TOX is the PDP-10 file that contains the TOX-SCREEN program. The SYS:ERF.REL refers to the error function that is needed by TOX-SCREEN.

During execution, TOX-SCREEN outputs results into seven separate output files using different logical output device numbers. Table 2 shows the logical output device numbers that are used in TOX-SCREEN. When executing TOX-SCREEN on the PDP-10, the results are output into files with names FOR06.DAT, FOR13.DAT, FOR14.DAT, FOR15.DAT, FOR16.DAT, FOR17.DAT, and FOR19.DAT. These output files are discussed further in Section 5.

The user can easily run the TOX-SCREEN computer code on the ORNL IBM 3033 computer by submitting the proper JCL. From a terminal at ORNL (connected to the PDP-10), the user would type the following command:

```
IBM SCREEN.JCL↓
```

and the program would be executed on the local IBM 3033 computer. Here, SCREEN.JCL is a PDP-10 file containing the JCL. This file is included in Appendix B of this report.

Although the above explains how to run TOX-SCREEN only on ORNL computers, users should have no problem implementing the code on other computers by using similar procedures.

4.2 INPUT DATA FILES

The following subsections discuss in detail how the input data files should be constructed by the user. Tables 3-9, included at the end of this section, will aid the user in preparing input files. Sample input data files are given in Appendix C. Briefly, the input for the SESOIL portion of TOX-SCREEN is read first by the program. TOX-SCREEN then reads the files containing the model flags, the air parameters, the water parameters, and the bioaccumulation parameters. Preparation of these files is discussed in the following subsections in the order that they are read by the TOX-SCREEN program.

Four types of standard FORTRAN format codes appear in Tables 3-9, the I, F, E, and A formats. The I format code is for integer data, the F and E

Table 2. Logical Output Device Numbers in TOX-SCREEN

Device Number	ORNL PDP-10 Data File	Data Description
6	FOR06.DAT	Contains output from SESOIL portion of TOX-SCREEN (Bonazountas and Wagner, 1981).
13	FOR13.DAT	The input data to TOX-SCREEN are written into this file so the user can determine if they were input correctly. Also, any error messages are written into this file.
14	FOR14.DAT*	Contains results from a simulation when the water body is a lake or for soil-air interaction only.
15	FOR15.DAT*	Contains results from a simulation when the water body is a river.
16	FOR16.DAT*	Contains results from a simulation when the water body is an estuary.
17	FOR17.DAT*	Contains results from a simulation when the water body is an ocean.

Table 2. (Continued)

Device Number	ORNL PDP-10 Data File	Data Description
19	FOR19.DAT	Contains output from the food chain bioaccumulation subroutine BIOCHN.

---

*These files are not written if the particular corresponding water body is not considered in the simulation. If no water body is considered at all (soil-air interaction only), results are written into FOR14.DAT.

format codes are used in transmitting real data, and the A format code is used in transmitting data that is in character format. For the I, E, and F formats, leading, embedded, and trailing blanks in a field of the input card are interpreted as zeros. Thus, when no decimal is present in the input data item, the item must be right justified in its field. If the decimal point is present (F or E format), its position overrides the position indicated by the d portion of the format field descriptor (Fw.d or Ew.d), and the number of positions specified by the w portion of this field must include a place for it. For E formats, the E may be omitted from the exponent if the exponent is signed (i.e., 1.0E+1 may be typed as 1.0+1).

4.2.1 SESOIL Input

Data for the SESOIL portion of the TOX-SCREEN program are read first. Arthur D. Little has compiled some generic input data for their SESOIL program (Bonazountas and Wagner, 1981). As mentioned in Section 3, the SESOIL subroutine RFILE adapted for TOX-SCREEN will read data for only the LEVEL3 mode of operation. However, TOX-SCREEN is capable of reading any existing SESOIL data files since it will skip over any LEVEL0, LEVEL1, or LEVEL2 data in the files until it reaches the appropriate LEVEL3 data. Thus, the user can either use existing SESOIL data compiled by A. D. Little (Bonazountas and Wagner, 1981) or put together his/her own data files. In either case, the step by step instructions given in Tables 3-5 must be followed carefully. Table 3 shows how to construct the SESOIL data file containing the executive (EXEC) data (see FOR05.DAT in Table 1 and Appendix C). This file controls the execution of the SESOIL portion of TOX-SCREEN as well as the reading of various SESOIL data files. While reading these tables, it will become clear that the file described in Table 3 is employed in conjunction with the data files described in Tables 4 and 5. One restriction applied to the EXEC data in Table 3 for TOX-SCREEN is that the parameter JRUN must be 1. That is, only one run can be made at one time by the TOX-SCREEN program whereas in the original SESOIL program an unlimited number of runs can be specified at one time. Note also that the parameter LEVEL must always be 3 specifying the LEVEL3 mode of operation. JYRS, the number of years to be simulated, must be $\leq$ 10.

The SESOIL general (GE) data file input sequence is described in Table 4 (see FOR01.DAT in Table 1 and Appendix C). Information contained in this file includes regional descriptions, soil classifications, and chemistry data. This file has been described in detail in Bonazountas and Wagner (1981). Table 4 describes what data is needed for the LEVEL3 mode of operation only. Data for other levels of operation (i.e., 0, 1, and 2) will not be discussed here since they are not used in TOX-SCREEN. One parameter has been added to this SESOIL file for use in TOX-SCREEN. Line 17 of Table 4 contains the added parameter RDUST, the dust loading parameter (McDowell-Boyer and Hetrick, 1982). If columns 67-73 of line 17 are left blank or are put to 0.0, then resuspension of dust particles from soil to air will not be considered. Thus, if existing SESOIL data are used, then this parameter should be added in the appropriate place in the file.

The SESOIL file described in Table 5 contains information required to perform a LEVEL3 (L3) application (see FOR02.DAT in Table 1 and Appendix C). The device number used to read this file was changed from 7 to 2 in the SESOIL portion of TOX-SCREEN since device number 7 is reserved for the card punch on the local ORNL PDP-10 computer. This file description has not changed from that documented in Bonazountas and Wagner (1981). Note that if there is no direct pollutant application to the soil, the parameter AR (surface area) should be set to 0.0 (see line 2). In this case, TOX-SCREEN computes the soil area that receives pollutant deposition from the air.

4.2.2 Model Flags

Section 3.2 discussed the numerous options available to the user in running the TOX-SCREEN code. Table 6 discusses the model flags which determine what options are chosen (see FOR10.DAT in Table 1 and Appendix C). If the user desires interactions between only the air and soil compartments, then the flags LAKE, RIVER, ESTU, and OCEAN should all be set to NO signifying a water body is not being considered in the simulation. Of course, any combination of YES or NO can be used for the flags LAKE, RIVER, ESTU, and OCEAN. This file is employed in connection with the data files described in Tables 7 and 8. For example, if the parameter LAKE is set to YES but SEDLKE is set to NO, then the user must follow the instructions for the parameter TRICON. The input data are different, depending on whether TRICON is set to YES or NO as explained in Table 8.

4.2.3 Air Parameters

The file that contains the air parameters is described in Table 7 (see FOR11.DAT in Table 1 and Appendix C). This file is not needed if the parameter OCEAN in Table 6 is set to YES while the parameters LAKE, RIVER, and ESTU are all NO since media interactions between coastal waters and air or soil are not considered. Otherwise, the first three data cards are always required. Notice that thereafter different input data are required depending on whether the parameter AIRFLG from Table 6 is POIN, AREA, or NONE. For simplicity of illustration, Table 7 assumes that the parameter JYRS from Table 3 is 1. For example, as discussed in Table 7, if JYRS>1, then the number of cards needed for the UW(MON,IYR) will depend on the number of years selected. For more information regarding default values for parameters in Table 7, see McDowell-Boyer and Hetrick (1982).

4.2.4 Water Parameters

Table 8 describes the input sequence needed in compiling the file of water parameters (see FOR12.DAT in Table 1 and Appendix C). This file can be ignored if all the flags LAKE, RIVER, ESTU, and OCEAN are set to NO (see Table 6). However, if any of these parameters are set to YES, step by step instructions are given in Table 8. In this case, card 1 is always needed. Thereafter, the data depend on whether the parameters LAKE, RIVER, ESTU, and OCEAN are set to YES or NO. Again, for simplicity of illustration, Table 8 assumes that the parameter JYRS from Table 3 is 1. Default values for many of the parameters in Table 8 are given in McDowell-Boyer and Hetrick (1982).

Some points given in Table 8 need further clarification. In the case where the parameter LAKE is YES, SEDLKE is NO, and TRICON is YES (see cards 7_L - 8_L), then the user should set SEDCL(MON,IYR) to the average suspended sediment concentration in the tributary flowing into the lake for month MON and year IYR. TOX-SCREEN then uses this information to compute the suspended sediment concentration in the lake. However, if both SEDLKE and TRICON are set to NO, then the tributary parameters DIASDT, DENSDT, DENWT, WDEPT, and SLOPET (see card 7_L) are used to estimate the sediment concentration in the tributary and this value is then used to determine the sediment concentration in the lake. Likewise, if RIVER is YES but SEDRIV is NO (see card 8_R), the user inputs parameters DIASDR, DENSDR, DENWR, and SLOPER which are used to compute the sediment concentration in the river (see subsection 3.4.2). For estuaries, if ESTU is set to YES and if the longitudinal dispersion coefficient EL is not known (DISFLG set to NO), parameter TIDMAX (maximum tidal velocity) can be input (see card 6_E). TOX-SCREEN will use TIDMAX to compute a longitudinal dispersion coefficient (see McDowell-Boyer and Hetrick, 1982).

4.2.5 Bioaccumulation Parameters

The input sequence for the bioaccumulation parameters is described in Table 9 (see FOR18.DAT in Table 1 and Appendix C). Default values for parameters in Table 9 are given in the discussion in Appendix F. Note that line 2 of this file is not needed if the parameter COVFLG in line 1 is set to YES.

Table 3. SESOIL EXEC Data File Input Sequence

Card (or Line)	Format	Parameter Name	Type	Column Position	Definitions and Comments
1	(8I5)	JRUN	Integer	1-5 (right justified)	JRUN is the incremental number of the run. For the TOX-SCREEN program, this number should always be 1 since only one run can be made at one time. Type the number 1 in column 5.
		LEVEL	Integer	6-10 (right justified)	LEVEL is the SESOIL level of operation. For TOX-SCREEN, LEVEL is always 3. Type the number 3 in column 10.
		JRE	Integer	11-15 (right justified)	JRE is the index of the region of interest. The user should match JRE with NRE from Table 4. The last digit of this number should be typed in column 15 (i.e., the number must be right justified).
		JSO	Integer	16-20 (right justified)	JSO is the index of the soil type of interest. The user should match JSO with NSO from Table 4. The last digit of this number should be typed in column 20.
		JCH	Integer	21-25 (right justified)	JCH is the index of the chemical compound of interest. The user should match JCH with NCH from Table 4. The last digit of this number should be typed in column 25.

Table 3. (Continued)

Card (or LINE)	Format	Parameter Name	Type	Column Position	Definitions and Comments
		JNUT	Integer	26-30 (right justified)	JNUT is the index for the nutrient cycle participation. This parameter is not used in the present model but it is reserved for later use. Leave as blank or enter 0 in column 30.
		JAPPL	Integer	31-35 (right justified)	JAPPL is the index for the application area of interest. The user should match JAPPL with NTY from Table 5. The last digit of this number should be typed in column 35.
		JYRS	Integer	36-40 (right justified)	JYRS is the number of years to be simulated. The user should make sure that JYRS is never greater than the number of years of data that is included in the data files discussed in Tables 4, 5, 7, and 8. The last digit of this number must be typed in column 40. JYRS must be ≤ 10 for dimensioning reasons.
2	(I5)	JRUN	Integer	1-5 (right justified)	Type the number 999 for JRUN in columns 3-5 to indicate the end of this file. When the program recognizes JRUN to be 999, it immediately ends execution.

Table 4. SESOIL GM Data File Input Sequence

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
1	(I1,5X,12A4)	NF	Integer	1	(-)	NF must be set to 1 here. It signifies that the data to follow describes the region of interest.
		TITLE	Character	7-54	(-)	TITLE can be the heading "REGIONAL DESCRIPTIONS; CLIMATIC STORM DATA" or any other heading the user desires. It is only used as a visual aid at the beginning of this file to indicate that climatic data follows.
2	(2X,I3,1X,12A4,I5)	NRE	Integer	3-5 (right justified)	(-)	NRE is the index of the site being considered. This number must match JRE (see Table 3) in order for the following data from this region to be used. The last digit of this number must be typed in column 5 (i.e., the number must be right justified).
		TITLES (1,12)	Character	7-54	(-)	TITLES(1,12) is the heading of the area or region where the model will be applied. This heading is written at the beginning of the output file for the user's convenience.
		IYRS	Integer	55-59 (right justified)	(-)	IYRS is the index of how many years of data follow. The last digit of this number must be typed in column 59. IYRS must be ≤ 10 because of dimensioning in the program.
3	(8X,1F6.2)	CLIMM1 (1,1,IYR) or L	Real	9-14 for IYR=1	°N	L is the latitude of the area (as a decimal). Columns 1-8 are ignored but can be used to identify the data.
4	(8X,12F6.2)	CLIMM1 (2,MON,IYR) or TA	Real	9-14 for MON=1,IYR=1 15-20 for MON=2,IYR=1 21-26 for MON=3,IYR=1 : 75-80 for MON=12,IYR=1	°C	CLIMM1(2,MON,IYR) is the temperature of the area for month MON and year IYR. MON=1 signifies the month October, MON=12 signifies September. Within the program, the parameter TA is set to CLIMM1(2,MON,IYR) for clarity.
5	(8X,12F6.2)	CLIMM1 (3,MON,IYR) or NN	Real	9-14 for MON=1,IYR=1 15-20 for MON=2,IYR=1 21-26 for MON=3,IYR=1 : 75-80 for MON=12,IYR=1	(fraction)	CLIMM1(3,MON,IYR) or NN is the fraction of sky covered by clouds for month MON and year IYR.
6	(8X,12F6.2)	CLIMM1 (4,MON,IYR) or S	Real	9-14 for MON=1,IYR=1 15-20 for MON=2,IYR=1 21-26 for MON=3,IYR=1 : 75-80 for MON=12,IYR=1	(fraction)	CLIMM1(4,MON,IYR) or S is the relative humidity of the area for month MON and year IYR.
7	(8X,12F6.2)	CLIMM1 (5,MON,IYR) or A	Real	9-14 for MON=1,IYR=1 15-20 for MON=2,IYR=1 21-26 for MON=3,IYR=1 : 75-80 for MON=12,IYR=1	(-)	CLIMM1(5,MON,IYR) or A is the shortwave albedo of the surface for month MON and year IYR. Representative values for the variables on cards 3-7 for various locations in the U.S. can be found in Bonazountas and Wagner (1981).

Table 4. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
8	(8X,12F6.2)	CLIMM1 (6,MON,ITR) or REP	Real	9-14 for MON=1,ITR=1 15-20 for MON=2,ITR=1 21-26 for MON=3,ITR=1 : 75-80 for MON=12,ITR=1	cm/day	CLIMM1(6,MON,ITR) or REP is the evapotranspiration rate of the area for month MON and year ITR. If this line is left blank or 0.0's are entered, then the code will use the parameters L,TA, NN,S and A to compute REP. However if REP is known, enter the values on this line and the code will not estimate it from the parameters L,TA,NN,S and A.
9	(8X,12F6.2)	CLIMM2 (1,MON,ITR) or MPM	Real	9-14 for MON=1,ITR=1 15-20 for MON=2,ITR=1 21-26 for MON=3,ITR=1 : 75-80 for MON=12,ITR=1	cm	CLIMM2(1,MON,ITR) or MPM is the precipitation for month MON and year ITR.
10	(8X,12F6.2)	CLIMM2 (2,MON,ITR) or MTR	Real	9-14 for MON=1,ITR=1 15-20 for MON=2,ITR=1 21-26 for MON=3,ITR=1 : 75-80 for MON=12,ITR=1	days	CLIMM2(2,MON,ITR) or MTR is the mean time of each rain event for month MON and year ITR.
11	(8X,12F6.2)	CLIMM2 (3,MON,ITR) or MN	Real	9-14 for MON=1,ITR=1 15-20 for MON=2,ITR=1 21-26 for MON=3,ITR=1 : 75-80 for MON=12,ITR=1	(-)	CLIMM2(3,MON,ITR) or MN is the number of storm events during month MON of year ITR.
12	(8X,12F6.2)	CLIMM2 (4,MON,ITR) or MT	Real	9-14 for MON=1,ITR=1 15-20 for MON=2,ITR=1 21-26 for MON=3,ITR=1 : 75-80 for MON=12,ITR=1	days	CLIMM2(4,MON,ITR) or MT is the mean length of the rain season (i.e., days in a month). If it rains almost every 3-4 days in a week during the entire month, then consider the rain season to last the entire month and set MT to 365/12 ~ 30.3.
13	This is an empty line for visual purposes. It indicates the end of year ITR=1. If ITRS (see line 2) is greater than 1, then lines 14-24 of this file would be the same as lines 3-13 except ITR would be 2; lines 25-35 would include the data for the third year, etc. For clarity, this table assumes the number of years ITRS=1. Also, another set of data for a totally different region can follow here. That is, cards 2-13 can be repeated here for another region. Note that, in this case, the parameter NRE from card 2 would have to be a different number for each region given. For any particular computer run, the user would set JRE (see Table 3) to the region NRE of interest. However, for clarity, this table assumes that only one region is given.					
14	(I1,5X,12A4)	NF	Integer	1	(-)	NF must be set to 2 here. It signifies that the data to follow describes the soil of interest.
		TITLE	Character	7-54	(-)	TITLE can be the heading "SOIL CLASSIFICATIONS; SOIL, SEDIMENT DATA" or any other heading the user desires. It is only used as a visual aid at the beginning of this section to indicate that soil data follows.
15	(2X,I3,1X,12A4)	NSO	Integer	3-5 (right justified)	(-)	NSO is the index of the soil being considered. This number must match JSO (see Table 3) in order for the following data for this soil type to be used. The last digit of this number must be typed in column 5.
		TITLES (2,12)	Character	7-54	(-)	TITLES(2,12) is an alphanumeric title used to describe the soil type. This title is written at the beginning of the output file.

Table 4. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
16	(38X,6F7.2)	RS	Real	39-45	g/cm^3	RS is the soil density.
		K1	Real	46-52	cm^2	K1 is the soil intrinsic permeability (see card 17 below).
		C	Real	53-59	(-)	C is the soil disconnectedness index.
		N	Real	60-66	(-)	N is the effective soil porosity. Representative values for the variables K1, C, and N for various soil types can be found in Bonazountas and Wagner (1981).
		OC	Real	67-73	% oc	OC is the organic content of the soil.
		CC	Real	74-80	% cc	CC is the clay content of the soil. This datum is not presently used in the SESOIL code so can be left blank. Columns 1-38 are ignored but can be used in the file to identify the data. The parameters of this line are stored in the array SOIL1(6).
17	(38X,5F7.2)	CEC	Real	39-45	meq/100g soil (meq=milli equivalents)	CEC is the soil cation exchange capacity.
		K1U	Real	46-52	cm^2	K1U is the intrinsic permeability of the upper soil layer.
		K1M	Real	53-59	cm^2	K1M is the intrinsic permeability of the middle soil layer.
		K1L	Real	60-66	cm^2	K1L is the intrinsic permeability of the lower soil layer. It is noted here that if K1 (see card 16) and the set of K1U, K1M, and K1L are given, the program will ignore the latter values and will use the value of K1 for all layers. Thus, if K1U, K1M, and K1L are known, leave the entry for K1 on card 16 blank.
		RDUST	Real	67-73	ug soil/m^3	RDUST is the dust loading factor. This is the only parameter that has been added to the original SESOIL input files in the TOX-SCREEN application. Default values are given in McDowell-Boyer and Hetrick (1982). The parameters of this line are stored in array SOIL2(6).
Lines 15-17 can be inserted for an unlimited number of soils. The parameter NSO from card 15 would have to be a different number for each soil type. For any particular computer run, the user would set JSO (see Table 3) to the soil type NSO of interest. However, for clarity, this table assumes only one soil type is given.						
18	(I1,5X,12A4)	NF	Integer	1	(-)	NF must be set to 3 here. It signifies that the data to follow describes the chemical of interest.
		TITLE	Character	7-54	(-)	TITLE can be the heading "CHEMISTRY DATA" or any other heading the user desires. It is only used as a visual aid at the beginning of this section to indicate that chemistry data follows.

Table 4. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
19	(2X,I3,1X,12A4)	NCH	Integer	3-5 (right justified)	(-)	NCH is the index of the chemical being considered. This number must match JCH (see Table 3) in order for the following data for this chemical type to be used. The last digit of this number must be typed in column 5.
		TITLES(3,12)	Character	7-54	(-)	TITLES(3,12) is an alphanumeric title used to describe the chemical. This title is written at the beginning of the output file for the user's convenience.
20	(38X,6F7.2)	SL	Real	39-45	μg/ml	SL is the compound solubility in water.
		KOC	Real	46-52	(μg/goc)/(μg/ml)	KOC is the adsorption coefficient of the compound on organic carbon.
		DA	Real	53-59	cm^2/sec	DA is the diffusion coefficient in air.
		KDE	Real	60-66	day^{-1}	KDE is the biodegradation rate of the compound.
		H	Real	67-73	m^3atm/mol	H is Henry's law constant.
		K	Real	74-80	(μg/g)/(μg/ml)	K is the averaged adsorption coefficient for the compound on the soil. If K is not given, the program estimates it by using KOC and OC (from line 16). The parameters in this line can be estimated using methodologies described in Lyman, Reehl, and Rosenblatt (1982). Columns 1-38 are ignored but can be used in the file to identify the data. The parameters of this line are stored in array CHEM1(18)
21	(38X,5F7.2)	MWT	Real	39-45	g/mol	MWT is the molecular weight of the compound.
		VAL	Real	46-52	(-)	VAL is the valence of the compound.
		KNH	Real	53-59	day^{-1}	KNH is the neutral hydrolysis constant.
		KBH	Real	60-66	ℓ/(mol day)	KBH is the base hydrolysis constant.
		KAH	Real	67-73	ℓ/(mol day)	KAH is the acid hydrolysis constant. The parameters of this line are stored in array CHEM1(18).
22	(38X,3F7.2)	SK	Real	39-45	(-)	SK is the stability constant of the compound - ligand complex.
		B	Real	46-52	#	B is the number of moles of ligand per mole of compound complexed.
		MWTLIG	Real	53-59	g/mol	MWTLIG is the molecular weight of the ligand. The parameters of this line are stored in array CHEM1(18).

Lines 19-22 can be repeated for an unlimited number of chemicals. The parameter NCH from card 19 would have to be a different number for each chemical type. For any particular computer run, the user would set JCH (see Table 3) to the chemical NCH of interest. However, for clarity, this table assumes only one chemical is given.

23	(I1,5X,12A4)	NF	Integer	1	(-)	NF must be set to 9 here. It signifies that this is the last line of this data file.
		TITLE	Character	7-54	(-)	TITLE can be the heading "END OF FILE" or any other heading the user desires. It is only used as a visual aid to the user.

Table 5. SESOIL L3 Data File Input Sequence

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
1	(2X,I3,1X,12A4,I5)	NTY	Integer	3-5 (right justified)	(-)	NTY is the index of the region that the simulation will be applied to. This number must match JAPPL (see Table 3) in order for the following data from this region to be used. The last digit of this number must be typed in column 5 (i.e., the number must be right justified).
		TITLES(5,12)	Character	7-54	(-)	TITLES(5,12) contains the heading related to the region/application for which data follow.
		IYRS	Integer	55-59 (right justified)	(-)	IYRS is the index of how many years of data follow. The last digit of this number must be typed in column 59. IYRS must be ≤ 10 because of dimensioning in the program.
2	(38X,5F7.2)	AR	Real	39-45	cm^2	AR is the surface area of the soil that is being affected by direct pollutant application. If the chemical is not applied directly to the soil surface, put AR = 0.0.
		Z	Real	46-52	m	Z is the depth to the groundwater table for this application.
		DU	Real	53-59	cm	DU is the depth of the upper unsaturated soil zone for this application.
		DM	Real	60-66	cm	DM is the depth of the middle unsaturated soil zone.
		FRN	Real	67-73	(-)	FRN is the Freundlich equation exponent.
						Columns 1-38 on this line are ignored but can be used in the file to identify the data. The parameters of this line are stored in array GEOM(20).
3	(38X,3F7.2)	PH	Real	39-45	(-)	PH is the pH of the upper soil zone layer.
		A2PH	Real	46-52	(-)	A2PH is the ratio of pH for the middle to upper soil layer.
		APH	Real	53-59	(-)	APH is the ratio of pH for the lower to upper soil layers.
						The parameters of this line are stored in array GEOM(20).
4	(38X,6F7.2)	A2KDE	Real	39-45	(-)	A2KDE is the ratio of the biodegradation rate of the compound in the middle soil zone to the upper soil zone.
		AKDE	Real	46-52	(-)	AKDE is the ratio of the biodegradation rate of the compound in the lower soil zone to the upper soil zone.
		A2OC	Real	53-59	(-)	A2OC is the ratio of the organic carbon content of soil in the middle soil zone to the upper soil zone.
		AOC	Real	60-66	(-)	AOC is the ratio of the organic carbon content of soil in the lower soil zone to the upper soil zone.

Table 5. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
		A2CC	Real	67-73	(-)	A2CC is the ratio of the clay content of the soil in the middle soil zone to the upper soil zone.
		ACC	Real	74-80	(-)	ACC is the ratio of the clay content of the soil in the lower soil zone to the upper soil zone.
						The parameters of this line are stored in array GEOM(20).
5	(38X,2F7.2)	A2CEC	Real	39-45	(-)	A2CEC is the ratio of the cation exchange capacity in the middle soil zone to the upper soil zone.
		ACEC	Real	46-52	(-)	ACEC is the ratio of the cation exchange capacity in the lower soil zone to the upper soil zone.
6	(8X,12F6.2)	RUNM1(1,MON) or CUM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/ml	RUNM1(1,MON) or CUM is the concentration of the pollutant in the soil moisture of the upper zone in month MON. If an application is to start with an already polluted column, this concentration should be entered in the month before any loading is specified. (MON=1 signifies the month October.)
7	(8X,12F6.2)	RUNM1(2,MON) or CMM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/ml	RUNM1(2,MON) or CMM is the concentration of the pollutant in the soil moisture of the middle zone in month MON. If an application is to start with an already polluted column, this concentration should be entered in the month before any loading is specified.
8	(8X,12F6.2)	RUNM1(3,MON) or CLM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12		RUNM1(3,MON) or CLM is the concentration of the pollutant in the soil moisture of the lower zone in month MON. If an application is to start with an already polluted column, this concentration should be entered in the month before any loading is specified.
9	(8X,12F6.2)	RUNM1(4,MON) or POLINU	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM1(4,MON) or POLINU is the monthly pollution load (mass) per unit area (cm^2) entering the upper soil zone.
10	(8X,12F6.2)	RUNM1(5,MON) or POLINM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM1(5,MON) or POLINM is the monthly pollution load (mass) per unit area (cm^2) entering the middle soil zone.
11	(8X,12F6.2)	RUNM1(6,MON) or POLINL	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM1(6,MON) or POLINL is the monthly pollution load (mass) per unit area (cm^2) entering the lower soil zone.
12	(8X,12F6.2)	RUNM1(7,MON) or ISRM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	(-)	RUNM1(7,MON) or ISRM is the monthly index for pollutant appearance in surface runoff. Set RUNM1(7,MON) to 0.0 for no surface runoff participation, to 1.0 for full surface runoff participation, or to some number in between 0.0 or 1.0 for partial surface runoff participation.

Table 5. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
13	(8X,12F6.2)	RUNM2(1,MON) or ASL	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	(-)	RUNM2(1,MON) or ASL contains the monthly ratio of the concentration of pollution in rain to the maximum solubility in water. Since subroutine AIR of TOX-SCREEN passes the concentration in the rain to the SESOIL portion of the program, this parameter is no longer needed. Although this parameter is not needed in the TOX-SCREEN adaptation, this card is still read by the program so as to not alter the existing SESOIL data.
14	(8X,12F6.2)	RUNM2(2,MON) or TRANSU	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(2,MON) or TRANSU is the monthly amount of pollutant transformed (chemically, biologically, or other) in upper soil zone, and not accounted for by individually existing model processes.
15	(8X,12F6.2)	RUNM2(3,MON) or TRANSM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(3,MON) or TRANSM is the monthly amount of pollutant transformed (chemically, biologically, or other) in the middle soil zone, and not accounted for by individually existing model processes.
16	(8X,12F6.2)	RUNM2(4,MON) or TRANSL	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(4,MON) or TRANSL is the monthly amount of pollutant transformed (chemically, biologically, or other) in the lower soil zone, and not accounted for by individually existing model processes.
17	(8X,12F6.2)	RUNM2(5,MON) or SINKU	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(5,MON) or SINKU is the monthly amount of pollutant "lost" by processes not directly described by the model (e.g., plant uptake) in the upper soil zone.
18	(8X,12F6.2)	RUNM2(6,MON) or SINKM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(6,MON) or SINKM is the monthly amount of pollutant "lost" by processes not directly described by the model in the middle soil zone.
19	(8X,12F6.2)	RUNM2(7,MON) or SINKL	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(7,MON) or SINKL is the monthly amount of pollutant "lost" by processes not directly described by the model in the lower soil zone.
20	(8X,12F6.2)	RUNM2(8,MON) or LIGU	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(8,MON) or LIGU is the monthly ligand mass input to the upper soil zone.
21	(8X,12F6.2)	RUNM2(9,MON) or LIGM	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(9,MON) or LIGM is the monthly ligand mass input to the middle soil zone.
22	(8X,12F6.2)	RUNM2(10,MON) or LIGL	Real	9-14 for MON=1 15-20 for MON=2 21-26 for MON=3 : 75-80 for MON=12	μg/cm^2	RUNM2(10,MON) or LIGL is the monthly ligand mass input to the lower soil zone.

Table 5. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
Lines 6-22 are repeated IYRS (see line 1) times. This table assumes IYRS is 1 for simplicity. Lines 1-22 can be repeated for an unlimited number of site-applications. Note that, in this case, the parameter NTY from card 1 would have to be a different number for each site given. For any particular computer run, the user would set JAPPL (see Table 3) to the site NTY of interest. For clarity, this table assumes data for only one site is given.						
23	(I1,5X,12A4)	NF	Integer	1	(-)	NF must be set to 9 here; it signifies that this is the last line of this data file.
		TITLE	Character	7-54	(-)	Title can be the heading "END OF FILE" or any other heading the user desires. It is only used as a visual aid to the user.

Table 6. Model Flags Parameter Input Sequence

Card (or Line)	Format	Parameter Name	Type	Column Position	Definition
1	(A4,6X,A4)	AIRFLG	Character	1-4	Specifies the type of air source. Type POIN for a point source, AREA for an area source, and NONE if there is no air source.
		AIRPOL	Character	11-14 (right justified)	Specifies physical form of the pollutant. Type PART in columns 11-14 for a particulate or GAS in columns 12-14 for a gas. This parameter is ignored if AIRFLG is NONE.
2	(A4,6X,A4,6X,A4)	LAKE	Character	1-4 (right justified)	If a lake is being considered in the simulation, type YES in columns 2-4; if not, type NO in columns 3-4.
		SEDLKE	Character	11-14 (right justified)	This parameter is used only when LAKE is set to YES. If the lake suspended sediment concentration is known or can be estimated, type YES in column 12-14 and follow instructions in Table 8. If unknown, type NO in columns 13-14 and follow instructions for the parameter TRICON below.
		TRICON	Character	21-24 (right justified)	This parameter is used only when LAKE is set to YES and SEDLKE is set to NO. If the suspended sediment concentration of a tributary flowing into the lake is known, then type YES in columns 22-24 and follow instructions in Table 8. If unknown, type NO in columns 23-24.

Table 6. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Definition
3	(A4,6X,A4)	RIVER	Character	1-4 (right justified)	If a river is being considered in the simulation, type YES in columns 2-4; if not, type NO in columns 3-4.
		SEDRIV	Character	11-14 (right justified)	The parameter is used only when RIVER is set to YES. If the total suspended sediment concentration in the river is known, type YES in columns 12-14, and follow instructions in Table 8. Otherwise, type NO in columns 13-14.
4	(A4,6X,A4)	ESTU	Character	1-4 (right justified)	If an estuary is being considered in the simulation, type YES in columns 2-4; if not, type NO in columns 3-4.
		DISFLG	Character	11-14 (right justified)	This parameter is used only when ESTU is set to YES. If the longitudinal dispersion coefficient for the estuary is known, type YES in columns 12-14, and follow instructions in Table 8. If not known, type NO in columns 13-14 and follow instructions for inputting the variable TIDMAX (maximum tidal velocity) in Table 8.
5	(A4)	OCEAN	Character	1-4 (right justified)	If an ocean is being considered in the simulation, type YES in columns 2-4; if not, type NO in columns 3-4.
6	(A4)	CHMFLG	Character	1-4	This card is ignored if the parameters LAKE, RIVER, ESTU, and OCEAN all are set to NO. However, if any of them are set to YES, then type ACID if the chemical is an acid, BASE if the chemical is a base, and NONE if the chemical is neither.

Table 7. Air Parameters Input Sequence

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definition and Comments
1	(20X,6E10.3)	UW(MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	m/s	UW(MON,IYR) is the wind speed for month MON and year IYR. MON=1 signifies the month October. Columns 1-20 are ignored but can be used to identify the data. If JYRS>1 (JYRS = number of years - see Table 3), then cards 3 and 4 would include UW(MON,IYR) for the second year, cards 5 and 6 would include UW(MON,IYR) for the third year, etc. This table assumes JYRS=1 for simplicity.
2	(20X,6E10.3)	UW(MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	m/s	
3	(20X,3E10.3)	UDG	Real	21-30	m/s	This card is always needed. UDG is the dry deposition velocity for gases. A default value is given in McDowell-Boyer and Hetrick (1982).
		WRATG	Real	31-40	(-)	WRATG is the washout ratio for gases. WRATG may be estimated by $1/H_c$ where H_c (M/M) is Henry's constant (McDowell-Boyer and Hetrick, 1982).
		AK	Real	41-50	s^{-1}	AK is the chemical degradation rate in air.
4	(20X,6E10.3)	QS(MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/s	Cards 4-10 are not needed if AIRFLG is set to NONE (see Table 6). However, if AIRFLG is either AREA or POIN, then QS(MON,IYR) is the pollutant source rate for month MON and year IYR. Again, as above, cards 6 and 7 would include QS(MON,IYR) for IYR=2 if JYRS=2, etc., but this table assumes JYRS=1 for simplicity.
5	(20X,6E10.3)	QS(MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/s	
If AIRFLG is set to AREA, then line 6 would be:						
6	(20X,1E10.3)	CTYLTH	Real	21-30	m	Do not include this line unless AIRFLG is set to AREA (see Table 6). CTYLTH is the length of the city or urban area - the area is assumed to be square.
If AIRFLG is set to POINT, then lines 6, 7, and 8 would be:						
6	(20X,6E10.3)	HMIX(MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	m	Do not include lines 6-8 unless AIRFLG is set to POIN (see Table 6). HMIX(MON,IYR) is the mixing height for month MON and year IYR. JYRS as defined in Table 3 is 1 here for simplicity. (If JYRS=2, cards 8 and 9 would be HMIX(MON,IYR) for the second year, etc.).

Table 7. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definition and Comments
7	(20X,6E10.3)	HMIX(MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	m	
8	(20X,6E10.3)	HS	Real	21-30	m	HS is the stack height. Again, do not include this line unless AIRFLG is set to POIN.
		VG	Real	31-40	m/s	VG is the gravitational settling velocity of the pollutant. Set VG to 0.0 if data are unavailable.
		VS	Real	41-50	m/s	VS is the stack gas exit velocity.
		SRAD	Real	51-60	m	SRAD is the stack radius.
		RHO	Real	61-70	kg/m^3	RHO is the stack gas density.
		ENTPY	Real	71-80	j/kg	ENTPY is the enthalpy of the stack gas. Although values of RHO and ENTPY for various gases are given in McDowell-Boyer and Hetrick (1982), if RHO and ENTPY can not be determined for the pollutant in question, just leave them blank and TOX-SCREEN will estimate the buoyancy flux parameter F (McDowell-Boyer and Hetrick, 1982, and Briggs, 1969) as G*VS*SRAD*SRAD where G is 9.8 m/s^2.
The next line would be card 7 if AIRFLG is AREA, card 9 if AIRFLG is POIN:						
7 or 9	(20X,2E10.3)	UDP	Real	21-30	m/s	This card is included only if AIRPOL is set to PART and AIRFLG is either AREA or POIN. UDP is the dry deposition velocity for the particulates.
		WRATP	Real	31-40	(-)	WRATP is the washout ratio for the particulates. Default values are given in McDowell-Boyer and Hetrick (1982).
10	(20X,1E10.3)	XLENS	Real	21-30	m	This card is needed only when AIRFLG is set to POIN and all the flags LAKE, RIVER, ESTU, and OCEAN are set to NO (see Table 6), signifying that no water body is being considered. XLENS is the length of the plume considered over the soil.

Table 8. Water Parameters Input Sequence*

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
1	(20X,2E10.3)	BISK	Real	21-30	moles/l	BISK is the acid or base dissociation constant. If CHMFLG (see Table 6) is ACID, then BISK is K_a = $[H^+]$ $[R^-]/[HR]_1$. If CHMFLG is BASE, then BISK is K_b = $[OH^-]$ $[HR]_1/[R^-]$ (McDowell-Boyer and Hetrick, 1982). $[HR]_1$ is the undissociated concentration (mol/l) of the neutral form and the concentrations of H^+, OH^-, and R^- are in mol/l.

The next section of data, cards 1_L - 6_L, will follow card 1 if LAKE is set to YES (see Table 6). However, ignore cards 1_L - 6_L if LAKE is set to NO.

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
1_L	(20X,6E10.3)	WCINL (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/s	WCINL(MON,IYR) is the pollutant source rate into the lake for month MON and year IYR. MON=1 signifies the month October. If JYRS>1 (JYRS=number of years - see Table 3) then cards 3_L and 4_L would include WCINL(MON,IYR) for the second year, etc. This table assumes JYRS=1 for simplicity.
2_L	(20X,6E10.3)	WCINL (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/s	
3_L	(20X,6E10.3)	WVELL (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	m/s	WVELL(MON,IYR) is the average velocity of the water flowing out of the lake for month MON and year IYR. That is, compute WVELL(MON,IYR) as Q_f /A/V, where Q_f = flow rate out of the lake (m^3/s), A = surface area of lake (m^2), and V = volume of lake (m^3). Again, this table assumes the number of years JYRS=1 for simplicity.
4_L	(20X,6E10.3)	WVELL (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	m/s	
5_L	(20X,4E10.3)	AREALK	Real	21-30	m^2	AREALK is the surface area of the lake.
		WDEPL	Real	31-40	m	WDEPL is the average water depth of the lake.
		XSOIL	Real	41-50	m	XSOIL is the distance of the far edge of the watershed from the lake. This parameter is input only when there is a point source (AIRFLG is set to POIN - see Table 6).
		HPLUSL	Real	51-60	moles/l	HPLUSL is $[H^+]$ for the lake. $[H^+] = 10^{-pH}$; for pH=7, $[H^+]$ = 1.0E-7. Areas of some lakes and drainage basins in the United States are given in McDowell-Boyer and Hetrick (1982).
6_L	(20X,6E10.3)	WKPL	Real	21-30	s^{-1}	WKPL is the photolysis rate constant for the lake. Columns 1-20 are ignored but can be used to identify the data.
		WKHL	Real	31-40	s^{-1}	WKHL is the hydrolysis rate constant for the lake.
		WKOL	Real	41-50	s^{-1}	WKOL is the oxidation rate constant for the lake.
		WKBL	Real	51-60	s^{-1}	WKBL is the biodegradation rate constant for the lake.
		WKVL	Real	61-70	s^{-1}	WKVL is the volatilization rate constant for the lake. If not available, WKVL may be estimated by a method given in McDowell-Boyer and and Hetrick (1982).

*This table can be ignored if all the flags LAKE, RIVER, ESTY, and OCEAN are set to NO (see Table 6).

Table 8. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
		SWKSWL	Real	71-80	moles/kg/ moles/l	SWKSWL is the soil-water partition coefficient for the lake. SWKSWL may be estimated as (K_{oc} % oc)/100 where K_{oc} expresses adsorption on a unit organic carbon basis, and (% oc) is the percentage of organic carbon in the sediment (McDowell-Boyer and Hetrick, 1982). Methodologies for estimating the parameters on this line can be found in Lyman, Reehl, and Rosenblatt (1982).

If SEDLKE is YES, or if SEDLKE is NO and TRICON is YES (see Table 6), then cards 7_L - 8_L would be:

7_L	(20X,6E10.3)	SEDCL (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/m^3	When SEDLKE is set to YES, then SEDCL(MON,IYR) is the average suspended sediment concentration in the lake for month MON and year IYR. However, if SEDLKE is NO and TRICON is YES, then SEDCL(MON,IYR) is the average suspended sediment concentration in the tributary flowing into the lake for month MON and year IYR. Sediment concentrations in some U.S. lakes are given in McDowell-Boyer and Hetrick (1982).
8_L	(20X,6E10.3)	SEDCL (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/m^3	

If both SEDLKE and TRICON are set to NO (see Table 6), then card 7_L is as follows (there would be no card 8_L in this case):

7_L	(20X,5E10.3)	DIASDT	Real	21-30	mm	DIASDT is the median sediment diameter in the tributary that flows into the lake.
		DENSDT	Real	31-40	g/cm^3	DENSDT is the density of the sediment in the tributary.
		DENWT	Real	41-50	g/cm^3	DENWT is the density of the water in the tributary.
		WDEPT	Real	51-60	m	WDEPT is the average water depth of the tributary.
		SLOPET	Real	61-70	(-)	SLOPET is the slope of the tributary. Default or typical values for DIASDT, DENSDT, and SLOPET are given in McDowell-Boyer and Hetrick (1982).

The next section of data, cards 1_R - 9_R, will follow the above if RIVER is set to YES (see Table 6). However, ignore cards 1_R - 9_R if RIVER is set to NO.

1_R	(20X,6E10.3)	WMINR (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/s	WMIN(MON,IYR) is the pollutant source rate into the river for month MON and year IYR. MON=1 signifies the month October. If JYRS>1 (JYRS=number of years - see Table 3), then cards 3_R - 4_R would include WMINR(MON,IYR) for the second year, etc. Here, JYRS=1 for simplicity.
2_R	(20X,6E10.3)	WMINR (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/s	
3_R	(20X,6E10.3)	WVELR (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	m/s	WVELR(MON,IYR) is the average water velocity of the river for month MON and year IYR. Again, this table assumes the number of years JYRS=1 for simplicity.
4_R	(20X,6E10.3)	WVELR (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	m/s	

Table 8. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
5_R	(20X,I10)	NR	Integer	21-30 (right justified)	(-)	NR is the number of reaches that the river is broken into. The last digit of this number must be typed in column 30. This number must be $\leq$ 20 because of dimensioning in the program.
6_R	(20X,4E10.3)	WLENR	Real	21-30	m	WLENR is the length of each river reach. (TOX-SCREEN assumes all river reaches have the same dimensions).
		WWIDR	Real	31-40	m	WWIDR is the average width of the river.
		WDEPR	Real	41-50	m	WDEPR is the average depth of the river.
		HPLUSR	Real	51-60	moles/l	HPLUSR is $[H^+]$ for the river. $[H^+] = 10^{-pH}$.
7_R	(20X,6E10.3)	WKPR	Real	21-30	s^{-1}	WKPR is the photolysis rate constant for the river. Columns 1-20 are ignored but can be used to identify the data.
		WKHR	Real	31-40	s^{-1}	WKHR is the hydrolysis rate constant for the river.
		WKOR	Real	41-50	s^{-1}	WKOR is the oxidation rate constant for the river.
		WKBR	Real	51-60	s^{-1}	WKBR is the biodegradation rate constant for the river.
		WKVR	Real	61-70	s^{-1}	WKVR is the volatilization rate constant for the river. If not available, WKVL may be estimated by a method given in McDowell-Boyer and Hetrick (1982).
		SWKSWR	Real	71-80	moles/kg/ moles/l	SWKSWR is the soil-water partition coefficient for the river. SWKSWR may be estimated as (K_{oc} % oc)/100 where K_{oc} expresses adsorption on a unit organic carbon basis, and (% oc) is the percentage of organic carbon in the sediment (McDowell-Boyer and Hetrick, 1982). Methodologies for estimating the parameters on this line can be found in Lyman, Reehl, and Rosenblatt (1982).

If SEDRIV is YES, then cards 8_R - 9_R would be (see Table 6):

8_R	(20X,6E10.3)	SEDCR (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/m^3	SEDCR(MON,IYR) is the average suspended sediment concentration in the river for month MON and year IYR. Again, JYRS=1 here for simplicity.
9_R	(20X,6E10.3)	SEDCR (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1		

Table 8. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
If SEDRIV is NO (see Table 6), then card 8_E is as follows (there would be no card 9_E in this case):						
8_E	(20X,4E10.3)	DIASDR	Real	21-30	mm	DIASDR is the median sediment diameter in the river bed.
		DENSDR	Real	31-40	g/cm^3	DENSDR is the sediment density in the river.
		DENWR	Real	41-50	g/cm^3	DENWR is the density of the water in the river.
		SLOPER	Real	51-60	(-)	SLOPER is the slope of the river bed. Default or typical values for DIASDR, DENSDR, and SLOPER are given in McDowell-Boyer and Hetrick (1982).
The next section of data, cards 1_E - 9_E, will follow the above if ESTU is set to YES (see Table 6). However, ignore cards 1_E - 9_E if ESTU is set to NO.						
1_E	(20X,6E10.3)	WMINE (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/s	WMINE(MON,IYR) is the pollutant source rate into the estuary for month MON and year IYR. MON=1 signifies the month October. If JYRS>1 (JYRS= number of years - see Table 3), then cards 3_E - 4_E would include WMINE(MON,IYR) for the second year, etc. Here, JYRS=1 for simplicity.
2_E	(20X,6E10.3)	WMINE (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/s	
3_E	(20X,6E10.3)	WVELE (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	m/s	WVELE(MON,IYR) is the fresh water velocity in the estuary for month MON and year IYR. Again, for clarity, the number of years JYRS=1 is assumed.
4_E	(20X,6E10.3)	WVELE (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	m/s	
5_E	(20X,I10)	NPTSE	Integer	21-30 (right justified)	(-)	NPTSE is the number of points both upstream and downstream of the pollutant source that TOX-SCREEN computes and outputs pollutant concentrations. The last digit of this number must be typed in column 30. This number must be ≤ 10 because of dimensioning in the program.
6_E	(20X,6E10.3)	WLENE	Real	21-30	m	WLENE is the length of the estuary.
		WWIDE	Real	31-40	m	WWIDE is the average width of the estuary.
		WDEPE	Real	41-50	m	WDEPE is the average depth of the estuary.
		EL	Real	51-60	m^2/s	EL is the longitudinal dispersion coefficient. If DISFLG is set to YES (see Table 6), then a value must be entered here. However, if DISFLG is set to NO, leave columns 51-60 blank.

Table 8. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
		TIDMAX	Real	61-70	m/s	TIDMAX is the maximum tidal velocity. This parameter is ignored unless DISFLG is set to NO.
		HPLUSE	Real	71-80	moles/1	HPLUSE is $[H^+]$ for the estuary. $[H^+] = 10^{-pH}$.
7_E	(20X,6E10.3)	WKPE	Real	21-30	s^{-1}	WKPE is the photolysis rate constant for the estuary. Columns 1-20 are ignored but can be used to identify the data.
		WKHE	Real	31-40	s^{-1}	WKHE is the hydrolysis rate constant for the estuary.
		WKOE	Real	41-50	s^{-1}	WKOE is the oxidation rate constant for the estuary.
		WKBE	Real	51-60	s^{-1}	WKBE is the biodegradation rate constant for the estuary.
		WKVE	Real	61-70	s^{-1}	WKVE is the volatilization rate constant for the estuary. If not available, WKVE may be estimated by a method given in McDowell-Boyer and Hetrick (1982).
		SWKSWE	Real	71-80	moles/kg/ moles/1	SWKSWE is the soil-water partition coefficient for the estuary. SWKSWE may be estimated as (K_{oc} % oc)/100 where K_{oc} expresses adsorption on a unit organic carbon basis, and (% oc) is the percentage of organic carbon in the sediment (McDowell-Boyer and Hetrick, 1982). Methodologies for estimating the parameters on this line can be found in Lyman, Reehl, and Rosenblatt (1982).
8_E	(20X,6E10.3)	SEDCE (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/m^3	SEDCE(MON,IYR) is the average suspended sediment concentration in the estuary for month MON and year IYR. Sediment concentrations in some U.S. estuaries are given in McDowell-Boyer and Hetrick (1982).
9_E	(20X,6E10.3)	SEDCE (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/m^3	

The next section of data, cards 1_o - 9_o, will follow the above if OCEAN is set to YES (see Table 6). However, ignore cards 1_o - 9_o if OCEAN is set to NO.

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
1_o	(20X,6E10.3)	WCINO (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 71-80 for MON=6,IYR=1	kg/m^3	WCINO(MON,IYR) is 0.02 times the concentration of the effluent to the ocean for month MON and year IYR. The dilution factor 0.02 assumes state-of-the-art engineering practices for ocean outfall designs (McDowell-Boyer and Hetrick, 1982; Morel et al., 1975). MON=1 signifies the month of October. If JYRS>1 (JYRS = number of years - see Table 3) then cards 3_o - 4_o would include WCINO(MON,IYR) for the second year, etc. This table assumes JYRS=1 for simplicity.
2_o	(20X,6E10.3)	WCINO (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/m^3	
3_o	(20X,6E10.3)	WVELO (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	m/s	WVELO(MON,IYR) is the ocean current velocity for month MON and year IYR. Again, JYRS=1 here for simplicity.

Table 8. (Continued)

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definitions and Comments
4_o	(20X,6E10.3)	WVELO (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	m/s	
5_o	(20X,3E10.3)	BO	Real	21-30	m	BO is the length of the line source, or the initial width of the effluent field. Default values are given in McDowell-Boyer and Hetrick (1982).
		XOCEAN	Real	31-40	m	XOCEAN is the distance between points in the ocean at which TOX-SCREEN computes and outputs pollutant concentrations.
		HPLUSO	Real	41-50	moles/l	HPLUSO is $[H^+]$ for the ocean. $[H^+] = 10^{-pH}$.
6_o	(20X,6E10.3)	WKPO	Real	21-30	s^{-1}	WKPO is the photolysis rate constant for the ocean. Columns 1-20 are ignored but can be used to identify the data.
		WKHO	Real	31-40	s^{-1}	WKHO is the hydrolysis rate constant for the ocean.
		WKOO	Real	41-50	s^{-1}	WKOO is the oxidation rate constant for the ocean.
		WKBO	Real	51-60	s^{-1}	WKBO is the biodegradation rate constant for the ocean.
		WKVO	Real	61-70	s^{-1}	WKVO is the volatilization rate constant for the ocean. If not available, WKVE may be estimated by a method given in McDowell-Boyer and Hetrick (1982).
		SWKSWO	Real	71-80	moles/kg/ moles/l	SWKSWO is the soil-water partition coefficient for the ocean. SWKSWO may be estimated as (K_{oc} % oc)/100 where K_{oc} expresses adsorption on a unit organic carbon basis, and (% oc) is the percentage of organic carbon in the sediment (McDowell-Boyer and Hetrick, 1982). Methodologies for estimating the parameters on this line can be found in Lyman, Reehl, and Rosenblatt (1982).
7_o	(20X,I10)	NPTSO	Real	21-30 (right justified)	(-)	NPTSO is the number of points from the pollutant source that TOX-SCREEN computes and outputs pollutant concentrations. The last digit of this number must be typed in column 30. NPTSO must be ≤ 10 because of dimensioning in the program.
8_o	(20X,6E10.3)	SEDCO (MON,IYR)	Real	21-30 for MON=1,IYR=1 31-40 for MON=2,IYR=1 41-50 for MON=3,IYR=1 51-60 for MON=4,IYR=1 61-70 for MON=5,IYR=1 71-80 for MON=6,IYR=1	kg/m^3	SEDCO(MON,IYR) is the average suspended sediment concentration in the ocean for month MON and year IYR. Again, JYRS=1 here for simplicity.
9_o	(20X,6E10.3)	SEDCO (MON,IYR)	Real	21-30 for MON=7,IYR=1 31-40 for MON=8,IYR=1 41-50 for MON=9,IYR=1 51-60 for MON=10,IYR=1 61-70 for MON=11,IYR=1 71-80 for MON=12,IYR=1	kg/m^3	

Table 9. Bioaccumulation Parameters Input Sequence

Card (or Line)	Format	Parameter Name	Type	Column Position	Units	Definition and Comments
1	(A4)	COVFLG	Character	2-4 (right justified)	(-)	Specifies whether the compound is or is not a covalently bonding material. Type NO in columns 3-4 if the compound is not a covalently bonding material and YES in columns 2-4 if it is. If COVFLG is YES, then ignore the rest of this table.
2	(20X,5E10.3)	KOW	Real	21-30	(-)	KOW is the n-octanol water partition coefficient. Methodologies for estimating K_{ow} can be found in Lyman, Reehl, and Rosenblatt (1982).
		R	Real	31-40	(-)	R is the initial interception fraction.
		YV	Real	41-50	g/m^2	YV is the productivity of terrestrial forage plants.
		LAMBDA	Real	51-60	day^{-1}	LAMBDA is the weathering constant.
		TE	Real	61-70	day	TE is the growth period of the terrestrial plants before harvest by grazing animals. Default or typical values for R, YV, LAMBDA, and TE can be found in Appendix F of this report.

5. DESCRIPTION OF CODE OUTPUT

Section 4 (Table 2) listed the different output files that can be written during TOX-SCREEN execution on the ORNL PDP-10 computer. This section gives a more detailed description of what is written into each output file. The reader is referred to Appendix D, which contains the TOX-SCREEN output that was written during execution of TOX-SCREEN using the sample input data from Appendix C.

5.1 OUTPUT FROM SESOIL PORTION OF TOX-SCREEN

Output from the SESOIL portion of TOX-SCREEN is written into a separate file (see file FOR06.DAT in Table 2 and Appendix D). The input data to SESOIL are written first so that the user can determine if they were input correctly. This section of the output is self-explanatory. The monthly results from SESOIL are given next for the first year of simulation. The hydrologic cycle components are written first. These results include monthly values for soil moisture, precipitation, net infiltration, evapotranspiration, surface runoff, and groundwater runoff. Next, the output states what kind of water body was considered in the simulation and the soil area next to the water body that has been contaminated. If, for example, the first water body considered was a lake, subsequent output would include results specific to the fact that the water body was a lake. These results include (1) the monthly pollutant mass input to the soil column, (2) the monthly pollutant mass distribution in the soil column (in surface runoff, volatilized, etc.), (3) the monthly pollutant concentration in the soil column (includes pollutant concentration in soil moisture (μg/ml), in soil adsorbed phase (μg/g), and in the soil air or vapor phase (μg/ml)), (4) the maximum depth that the pollutant reaches each month and (5) an annual summary report of the hydrologic cycle components and items (1) - (4). If the only water body considered in a simulation was a lake, then this file would end here.

Otherwise, results for the water body being a river (if considered) are given next, followed by results for the water body being an estuary (if considered).

The contaminated soil area is printed only for the first month in a simulation for each water body type considered. If there is a point source in the air compartment, this area could change slightly each month due to different monthly wind speeds, since the plume size determines contaminated soil area size.

No results are ever given in this file for oceans since at the present time TOX-SCREEN does not consider interaction with the soil compartment in this case. If no water body is considered in a particular simulation (i.e., soil-air interaction only), then before the results (1) - (5) above are printed, a message is written stating that no water body was included in the calculations. The contaminated soil area is printed also.

5.2 OUTPUT OF TOX-SCREEN INPUT DATA AND ERROR MESSAGES

A separate output file (see FOR13.DAT in Table 2 and Appendix D) contains tables of all input data (excludes SESOIL data). These tables enable the user to determine whether or not the data were input correctly. The first table written into this file contains information about the model flags. The computer name, the option chosen, and the definition are given for each model flag. Notice in the sample output of Appendix D that the flags LAKE, RIVER, ESTU, and OCEAN were all YES signifying that all four water bodies were considered in the sample computer run and different results were computed for each.

Following the model flags table is a table containing the input data for the air compartment parameters. For each air parameter, the computer name, definition, unit, and numerical value (or values if monthly) is given. If an ocean is the only water body considered in a simulation (i.e., LAKE, RIVER, and ESTU are NO, but OCEAN is YES), then this table is not printed since no air data are needed in this case.

A table containing the input data for the water compartment parameters is printed. Again, the computer names, definitions, units, and numerical values are given. At the beginning of this table, a constant is given that is not water body dependent. Next, water body dependent parameters are given. If any or all of the water bodies are not selected, corresponding sections of the table would not be written.

Following the water compartment parameters table is another table showing the types and magnitudes of the source terms. This table shows which compartments (air, water, soil) have sources, which water bodies are considered, the geographic region under consideration, and the monthly magnitudes for each source.

Where feasible, the TOX-SCREEN computer code checks the input data and if an error (an obviously illogical value or choice) is detected, a message is printed into this file (FOR13.DAT) and execution stops. For example, the parameter LAKE must be either YES or NO. If LAKE is input incorrectly, the following message will be written into this file: "ERROR IN DATA: LAKE DOES NOT EQUAL YES OR NO, BUT = ____", where ____ is the incorrect data. Numerous other checks such as this one can be found in the computer program. Also, some checks are made during actual execution of TOX-SCREEN (i.e., after the input data are read). If errors are detected, messages will be written into this file. Thus, the user should always check this output file (FOR13.DAT) very carefully, especially if execution stops prematurely.

5.3 OUTPUT WHEN WATER BODY IS A LAKE

A separate output file (see file FOR14.DAT in Table 2 and Appendix D) presenting results in all media is printed when a lake is specified as a water body being present in a TOX-SCREEN run. These results include monthly pollutant concentrations and media interaction terms. The contaminated surface area of the lake and soil area next to the lake are printed first. Thereafter, two lines of results are printed for each month. These two lines are labeled clearly. The first line contains pollutant concentrations in μg/m^3 for each compartment. These results include (from left to right) maximum and average air concentrations, water concentrations in the dissolved neutral, dissolved ionic, and adsorbed forms, soil concentrations in the upper, middle, and lower soil zones, and the pollutant concentration in air due to resuspension from soil. This latter concentration is included in the maximum and average air concentrations as well. If there is an atmospheric area source, asterisks are printed for maximum air concentration since TOX-SCREEN assumes that the maximum and average air concentrations are the same in this case (McDowell-Boyer and Hetrick, 1982).

The second line of results for each month contains the media interaction rates in μg/mon. These results include (from left to right) deposition rates from air to water and soil, volatilization rates from water and soil to air, surface and groundwater runoff from soil to water, and washload (erosion by water) from soil to water (see McDowell-Boyer and Hetrick, 1982).

This file (FOR14.DAT) is not written if the parameter LAKE is set to NO in the input data, providing any of the parameters RIVER, ESTU, or OCEAN are set to YES. However, if all the flags LAKE, RIVER, ESTU, and OCEAN are set to NO, signifying that TOX-SCREEN considers only soil-air interactions, then the results from such a simulation will be written into this file. This case is discussed further in Section 5.8 below.

5.4 OUTPUT WHEN WATER BODY IS A RIVER

As for the results when a lake is specified, TOX-SCREEN output for a river simulation are written into a separate file (see file FOR15.DAT in Table 2 and Appendix D). The output format for the river results is identical to that for the lake with the exception that the pollutant concentrations in the water are printed for each reach in the river (the number of reaches is specified by the user in the input data - see Table 8). As shown in the sample output in Appendix D, the reach number is identified by the computer name IR. This file is not written if the flag RIVER is set to NO (see Table 6).

5.5 OUTPUT WHEN WATER BODY IS AN ESTUARY

A separate output file is printed showing results when an estuary is considered (see file FOR16.DAT in Table 2 and Appendix D). Again, the output format for the estuary results is identical to that for the lake with the exception that the pollutant concentrations in the estuary are printed at different points both upstream and downstream of the source. The parameter X in this file is the distance from the source in meters. Values are given for points upstream and downstream of the source (-X is used for upstream and +X for downstream). The number of points at which concentrations are printed is specified by the user (see Table 8). This file will not be printed if the flag ESTU is specified by the user to be NO (see Table 6).

5.6 OUTPUT WHEN WATER BODY IS AN OCEAN

Since TOX-SCREEN does not consider interaction with the soil and air compartments when the water body is an ocean, the output file in this case (see file FOR17.DAT in Table 2 and Appendix D) contains only monthly concentrations in the water. Pollutant concentrations in the water are given in the dissolved neutral, dissolved ionic, and adsorbed forms at different distances from the source. The number of points from the source that TOX-SCREEN computes and outputs results and the distance between these points are specified by the user in the input data (see Table 8). This file is not written if the flag OCEAN is set to NO (see Table 6).

5.7 FOOD CHAIN BIOACCUMULATION OUTPUT

As mentioned in Section 3, the food chain bioaccumulation model has been added to the TOX-SCREEN code recently. Thus, the results (from subroutine BIOCHN) are written into a separate output file (see FOR19.DAT in Table 2 and Appendix D). Unlike the other output files, this file includes both a table of the input data for and a table of the results of the food chain bioaccumulation model. The food chain flag COVFLG and its definition are printed first. If this flag is input incorrectly, an error message is printed and execution stops. If this flag is input as YES, signifying that the compound is a covalently bonding compound, then the message "BIOACCUMULATION CANNOT BE ESTIMATED BY THE EMPLOYED METHOD" is printed. In this case, the model cannot be used and no other information is written (for more information, see Appendix F). However, if COVFLG is NO, then the input parameters for the food chain model are written next. For this case, as shown in Appendix D, the computer name, definition, unit, and value is given for each bioaccumulation parameter. A printout of the bioaccumulation factors (aquatic, plant, and animal) follows. These factors are discussed in Appendix F.

Next, a table of the monthly concentrations in aquatic organisms and terrestrial plants in μg/g is given. Two columns of numbers are given if the water body is a lake, river, or estuary; one for the monthly aquatic results and the other for the monthly plant results. For oceans, only monthly aquatic results are given since the soil compartment is not included in this case. If no water body is considered in the simulation (i.e., the flags LAKE, RIVER, ESTU, and OCEAN are NO), then results are given only for plants since TOX-SCREEN considers only soil-air interaction in this case. These results are given in the last column of this table. The results for the water bodies would all be zeros if this option is chosen. Likewise, if a particular water body is not considered, zeros are printed in the appropriate columns. A discussion of the methods used in computing the numbers in this table is included in Appendix F.

This output file ends with a caution note stating the limitations of the methods used in the food chain bioaccumulation model. These limitations are discussed further in Appendix F.

5.8 OUTPUT WHEN NO WATER BODY IS CONSIDERED

When TOX-SCREEN does not consider the water compartment (i.e., flags LAKE, RIVER, ESTU, and OCEAN are all set to NO), the results are written into file FOR14.DAT on the local PDP-10 computer (see Table 2). That is, the same unit output device number is used in this case as used for printing results when a lake is considered. The format of this output file is identical to that explained in subsection 5.3 above except that a message is printed that no water body is considered and, of course, the surface area of the water is not printed. Also, asterisks are printed under the columns for the water concentrations, the deposition rate on water, and the volatilization rate from water since these values are not included in this option. If there is an area air source, asterisks are printed for maximum air concentration since TOX-SCREEN assumes that the maximum and average air concentrations are the same in this case (McDowell-Boyer and Hetrick, 1982).

6. DISCUSSION

This report has provided a description of the TOX-SCREEN model, and subroutine structure of, input requirements and format for, and description of output from the TOX-SCREEN computer code. All of the subprograms of the TOX-SCREEN code (with the exception of the SESOIL portion of TOX-SCREEN) have been tested by doing preliminary stand-alone computer runs for each routine. For example, the results computed by subroutine WATER were checked by writing a driver routine that supplied WATER with the appropriate parameters. These results were compared to hand or calculator computations. Also, any changes made to the SESOIL portion of TOX-SCREEN were checked by making sure that results obtained after the changes were made were equal to the initial results. Once the subroutines were all put together to form TOX-SCREEN, numerous additional checks were made to insure the results were correct. Thus, much effort was put forth in checking and rechecking code calculations.

The input data (Appendix C) used for the sample computer run that produced the output in Appendix D were hypothetical. Default values were used for many of the input parameters (see McDowell-Boyer and Hetrick, 1982). It was the authors' intent to show the capabilities of the model through use of this example, not to show an actual application.

The assumptions used in the TOX-SCREEN model have been discussed in both this report and the companion report by McDowell-Boyer and Hetrick (1982). However, the user should be made aware of the following points when water bodies are considered. First, the treatment of bases assumes that the base is a negatively charged ion and that the ionization reaction is (McDowell-Boyer and Hetrick, 1982):

$$R^- + H_2O \rightleftharpoons RH + OH^- \ .$$

For example, if ammonia (NH_3) is input, the assumed ionization is:

$$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^- .$$

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TOX-SCREEN will report the concentration of ammonium ion [NH_4^+] as the concentration of its dissolved neutral species. Further, it will volatilize the ammonium ion rather than NH_3. Second, the user should be warned that ionized and adsorbed species are presumed not to undergo transformation reactions, that adsorption of ions via ionic exchange processes is neglected, and that capture of the chemical of concern by the resident bed sediments is ignored. The resident bed sediments, and toxicity to the benthic infauna, are of major concern in many TSCA evaluations. In some cases, neglect of the resident bed sediments is not a conservative assumption. The resident bed sediments will be considered in future work on the TOX-SCREEN model.

It is hoped that TOX-SCREEN can be used as a screening device in identifying chemicals that are highly unlikely to pose a problem even under conservative assumptions. Advances in understanding and prediction occur through the cycles of model development and applications. Preliminary results obtained from a TOX-SCREEN application with source data for trichloroethylene are encouraging. Applications and results will be documented in subsequent reports.

REFERENCES

1. Bagnold, R. A., An Approach to the Sediment Transport Problem from General Physics, Geological Survey Professional Paper 422-I, U.S. Government Printing Office (1966).

2. Bonazountas, M. and J. Wagner, SESOIL: A Seasonal Soil Compartment Model, Draft Report, Arthur D. Little, Inc., Cambridge, Mass., Prepared for the U.S. Environmental Protection Agency, Office of Toxic Substances (1981).

3. Briggs, G. A., Plume Rise, TID-25075, U.S. Atomic Energy Agency, Division of Technical Information (1969).

4. Brooks, N. H., "Diffusion of Sewage Effluent in an Ocean-Current," pp. 264-7 in Proceedings of the First International Conference on Waste Disposal in the Marine Environment, Pergamon Press (1960).

5. Browman, M. G. and G. Chesters, "The Solid-Water Interface: Transfer of Organic Pollutants Across the Solid-Water Interface," pp. 49-103 in Fate of Pollutants in the Air and Water Environments Part 1, Vol. 8, I. H. Suffet (ed.), John Wiley and Sons, Inc., New York.

6. Browman, M. G., M. R. Patterson, and T. J. Sworski, Formulations of the Physicochemical Processes in the ORNL Unified Transport (UTM-TOX), ORNL/TM-8013, Oak Ridge National Laboratory (1982).

7. Burns, L. A., D. M. Cline, and R. R. Lassiter, Exposure Analysis Modeling SYSTEM (EXAMS): User Manual and System Documentation, EPA-600/3-82-023, U.S. Environmental Protection Agency, Office of Research and Development (1982).

8. Chamberlain, A. C., "Interception and Retention of Radioactive Aerosols by Vegetation," Atmos. Environ. 4:57-78 (1970).

9. Fields, D. E., CHNSED: Simulation of Sediment and Trace Contaminant Transport with Sediment/Contaminant Interaction, ORNL/NSF/EATC-19, Oak Ridge National Laboratory (1976).

10. Forsythe, G. E., M. A. Malcolm, and C. B. Moler, Computer Methods for Mathematical Computations, Prentice-Hall, Inc. (1977).

11. Gifford, F. A., and S. R. Hanna, "Modeling Urban Air Pollution," Atmos. Environ. 7: 131-6 (1973).

12. Hanna, S. R., "A Stability Correction Term for a Simple Urban Dispersion Model," pp. 242-8 in preprints for the Joint Conference on Applications of Air Pollution Meteorology, Salt Lake City, November 29-December 2, 1977, American Meteorological Society, Boston, Mass. (1977).

13. Laursen, E. M., "The Total Sediment Load of Streams," Paper #1530 in Proceedings of ASCE 84, HY1 (1958).

14. Lyman, W. J., W. F. Reehl, ad D. H. Rosenblatt, Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company (1982).

15. McDowell-Boyer, L. M. and D. M. Hetrick, A Multimedia Screening-Level Model for Assessing the Potential Fate of Chemicals Released to the Environment, ORNL/TM-8334, Oak Ridge National Laboratory (1982).

16. Morel, F. M. M., J. C. Westall, C. R. O'Melia, and J. J. Morgan, "Fate of Trace Metals in Los Angeles County Wastewater Discharge," Environmental Science Technology 9(8): 756-61 (1975).

17. NAGFLIB - Numerical Algorithms Group FORTRAN Library Manual, MK8, January 1981.

18. Pasquill, F., "The Estimation of the Dispersion of Windborne Material," Meteorol. Mag. 90: 33 (1961).

19. Smith, J. H., W. R. Mabey, N. Bohonos, B. R. Holt, S. S. Lee, T. W. Chow, D. C. Bomberger, and T. Mill, Environmental Pathways of Selected Chemicals in Freshwater Systems, EPA 600/7-77-113, U. S. Environmental Protection Agency (1977).

20. U.S. Nuclear Regulatory Commission, Estimating Aquatic Dispersion of Effluents from Accidental and Routine Reactor Release for the Purpose of Implementing Appendix I, Revision 1, Regulatory Guide 1.113 (1977).

21. Zison, S. W., K. F. Haven, and W. B. Mills, Water Quality Assessment: A Screening Method for Nondesignated 208 Areas, EPA-600/9-77-023, U.S. Environmental Protection Agency, Office of Research and Development (1977).

APPENDIX A

IMPORTANT PARAMETERS AND THEIR DEFINITIONS

The parameters in this appendix are listed in alphabetical order. To save space, parameters that are similar are listed together. For example, the dissolved fraction α_1 is different for each water body, but the parameter names are A1? where ? is E for estuary, L for lake, O for ocean, and R for river. Parameters of this type are listed with only one definition in this appendix.

PARAMETER	DEFINITIONS	COMMON/SUBROUTINE
A1E A1L A1O A1R	Undissociated dissolved fraction α_1, for estuary, lake, ocean and river, respectively.	COMMON/ALPHAS/
A2E A2L A2O A2R	Dissolved ionic fraction α_2 for estuary, lake, ocean, and river, respectively.	COMMON/ALPHAS/
A3E A3L A3O A3R	Fraction adsorbed to sediment α_3 for estuary, lake, ocean, and river, respectively.	COMMON/ALPHAS/
ACMAXE ACMAXL ACMAXR ACMAXS	Maximum air concentration calculated in $\mu g/m^3$ when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
AIRFLG	Specifies the type of air source. AIRFLG = POIN implies point source, = AREA implies area source, and = NONE implies there is no air source.	COMMON/FLAGS/

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AIRPOL	Specifies the physical form of the pollutant. AIRPOL = PART implies particulate and = GAS implies gas.	COMMON/FLAGS/
AK	Chemical degradation rate in air in s^{-1}.	COMMON/AIRPAR/
ARE	Surface area of the soil in cm^2 affected by pollutant contamination when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/SPARE/
ARL		COMMON/SPARL/
ARR		COMMON/SPARR/
ARS		COMMON/SPARS/
AREA1(IWATER)	Contaminated soil area (first month) in m^2 next to lake if IWATER=1, river if IWATER=2, and estuary if IWATER=3.	COMMON/OUT/
AREAE	Surface area in m^2 of estuary, lake, and river, respectively.	COMMON/WPARE/
AREALK		COMMON/WPARL/
AREAR		COMMON/WPARR/
AREAPL	Area of plume (from point source) in m^2 over lake and soil next to water body, respectively.	SUBROUTINE AIR
AREAPS		
AREAS	Surface area of the soil in m^2 affected by pollutant contamination when soil (i.e., no water body), estuary, lake, and river option, respectively, is considered.	COMMON/SPARS/
AREASE		COMMON/SPARE/
AREASL		COMMON/SPARL/
AREASR		COMMON/SPARR/

ARPLS	Area in m^2 of plume (from point source) over the soil when no water body is considered.	SUBROUTINE AIR
ARSPLU	Surface area of the soil in cm^2 affected by pollutant contamination.	SUBROUTINE TRANS3
ASDEPE ASDEPL ASDEPR ASDEPS	Total deposition from air to soil in μg/mon when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
ASMIDE ASMIDL ASMIDR ASMIDS	Dry deposition in $kg/m^2/s$ from air to soil when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
ASMIND ASMINW	Dry and wet deposition, respectively, from air to soil in $\mu g/cm^2/mon$.	SUBROUTINE TRANS3
ASMIWE ASMIWL ASMIWR ASMIWS	Wet deposition in $kg/m^2/s$ from air to soil when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
ASMODE ASMODL ASMODR	Dry deposition in $kg/m^2/s$ from air to soil that will be used in the next time step when	COMMON/MEDIA/

ASMODS	estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	
ASMOWE ASMOWL ASMOWR ASMOWS	Wet deposition in kg/m^2/s from air to soil that will be used in the next time step when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
AVAIRE AVAIRL AVAIRR AVAIRS	Average air concentration in µg/m^3 when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
AVCNES AVCNRS AVCNS	Average concentration in air in kg/m^3 due to point source plume over estuary and soil, river and soil, and soil (i.e., no water body considered), respectively.	SUBROUTINE AIR
AVCONL AVCONS	Average concentration in air in kg/m^3 due to point source plume over lake, and soil next to lake, respectively.	SUBROUTINE AIR
AVCSL	Average concentration in air in kg/m^3 due to point source plume when a lake is considered. AVCSL = (AVCONL + AVCONS)/2.0.	SUBROUTINE AIR

AWDEPE AWDEPL AWDEPR	Total deposition from air to water in μg/mon when estuary, lake, and river option, respectively, is considered.	COMMON/OUT/
AWMINE AWMINL AWMINR	Total deposition from air to water (m_{in}) in kg/s when estuary, lake, and river option, respectively, is considered.	COMMON/MEDIA/
AWMOUE AWMOUL AWMOUR	Total deposition in kg/s from air to water (m_{out}) that will be used in the next time step when estuary, lake, and river option, respectively, is considered.	COMMON/MEDIA/
BCFAQ BCFPL	BCFAQ in ml/g is the ratio between concentration in tissue (fresh weight) and concentration in water. BCFPL is the ratio between concentration in tissue (dry weight) and concentration in soil and is unitless.	SUBROUTINE BIOCHN
BFUNC	Array used to store the cubic coefficients b_i (Forsythe, et al., 1977) needed in spline calculation of Laursen's function (Laursen, 1958).	SUBROUTINE FUNLAU
BO	Length of the line source in m for an ocean simulation.	COMMON/WPARO/

BP	Array used to store the cubic coefficients b_i (Forsythe, et al., 1977) needed in spline calculation of trapping efficiency P for lakes (Zison et al., 1977).	SUBROUTINE SEDCON
BTHETA	Array used to store the cubic coefficients b_i (Forsythe, et al., 1977) needed in spline calculation of Shields factor (Bagnold, 1966).	SUBROUTINE FUNLAU
BVFALL	Array used to store the cubic coefficients b_i (Forsythe, et al., 1977) needed in spline calculation of the fall velocity (Fields, 1976).	SUBROUTINE FUNLAU
C	C is a dimensionless parameter used in the area source model which is a function of stability and area size (McDowell-Boyer and Hetrick, 1982).	SUBROUTINE AIR
CFUNC	Array used to store the cubic coefficients c_i (Forsythe, et al., 1977) needed in spline calculation of Laursen's function (Laursen, 1958).	SUBROUTINE FUNLAU

CHEM1(1)	CHEM1(1) or SL is the compound solubility in water in μg/ml.	COMMON/CH/
CHEM1(2)	CHEM1(2) or KOC is the adsorption coefficient of the compound on organic carbon in (μg/goc)/(μg/ml).	COMMON/CH/
CHEM1(3)	CHEM1(3) or DA is the diffusion coefficient in air in cm^2/s.	COMMON/CH/
CHEM1(4)	CHEM1(4) or KDE is the biodegradation rate of the compound in day^{-1}.	COMMON/CH/
CHEM1(5)	CHEM1(5) or H is Henry's law constant in m^3 atm/mol.	COMMON/CH/
CHEM1(6)	CHEM1(6) or K is the averaged adsorption coefficient for the compound on the soil in (μg/g)/(μg/ml).	COMMON/CH/
CHEM1(7)	CHEM1(7) or MWT is the molecular weight of the compound in g/mol.	COMMON/CH/
CHEM1(8)	CHEM1(8) or VAL is the valence of the compound and is unitless.	COMMOM/CH/
CHEM1(9)	CHEM1(9) or KNH is the neutral hydrolysis constant in day^{-1}.	COMMON/CH/

CHEM1(10)	CHEM1(10) or KBH is the base hydrolysis constant in 1/(mol day).	COMMON/CH/
CHEM1(11)	CHEM1(11) or KAH is the acid hydrolysis constant in 1/(mol day).	COMMON/CH/
CHEM1(13)	CHEM1(13) or SK is the stability constant of the compound-ligand complex.	COMMON/CH/
CHEM1(14)	CHEM1(14) or B is the number of moles of ligand per mole of compound complexed.	COMMON/CH/
CHEM1(15)	CHEM1(15) or MWTLIG is the molecular weight of the ligand in g/mol.	COMMON/CH/
CHMFLG	This flag is equal to ACID if the chemical is an acid, BASE if the chemical is a base, and NONE if the chemical is neither.	COMMON/FLAGS/
CLIMM1(1,1,IYR)	CLIMM1(1,1,IYR) or L is the latitude in °N of the area.	COMMON/HYM/
CLIMM1(2,MON,IYR)	CLIMM1(2,MON,IYR) or TA is the temperature in °C of the area for month MON and year IYR.	COMMON/HYM/
CLIMM1(3,MON,IYR)	CLIMM1(3,MON,IYR) or NN is the fraction of sky covered by clouds for month MON and year IYR.	COMMON/HYM/

CLIMM1(4,MON,IYR)	CLIMM1(4,MON,IYR) or S is the relative humidity of the area for month MON and year IYR.	COMMON/HYM/
CLIMM1(5,MON,IYR)	CLIMM1(5,MON,IYR) or A is the shortwave albedo of the surface for month MON and year IYR.	COMMON/HYM/
CLIMM1(6,MON,IYR)	CLIMM1(6,MON,IYR) or REP is the evapotranspiration rate of the area in cm/day for month MON and year IYR.	COMMON/HYM/
CLIMM2(1,MON,IYR)	CLIMM2(1,MON,IYR) or MPM is the precipitation in cm for month MON and year IYR.	COMMON/HYM/
CLIMM2(2,MON,IYR)	CLIMM2(2,MON,IYR) or MTR is the mean time of each rain event in days for month MON and year IYR.	COMMON/HYM/
CLIMM2(3,MON,IYR)	CLIMM2(3,MON,IYR) or MN is the number of storm events during month MON of year IYR.	COMMON/HYM/
CLIMM2(4,MON,IYR)	CLIMM2(4,MON,IYR) or MT is the mean length of the rain season in days for month MON of year IYR.	COMMON/HYM/
CLM	Pollutant concentration in the soil moisture of the lower soil zone in μg/ml.	SUBROUTINE TRANS3

CLMEST CLMLKE CLMRIV CLMS	Pollutant concentration in the soil moisture of the lower soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
CLSA	Pollutant concentration in the the soil air of the lower soil zone in μg/ml.	SUBROUTINE TRANS3
CLSAES CLSALK CLSARV CLSAS	Pollutant concentration in the soil air of the lower soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
CMM	Pollutant concentration in the soil moisture of the middle soil zone in μg/ml.	SUBROUTINE TRANS3
CMMEST CMMLKE CMMRIV CMMS	Pollutant concentration in the soil moisture of the middle soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
CMSA	Pollutant concentration in the soil air of the middle soil zone in μg/ml.	SUBROUTINE TRANS3

CMSAES CMSALK CMSARV CMSAS	Pollutant concentration in the soil air of the middle soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
CNCED1(IE) CNCED2(IE) CNCED3(IE) CNCEU1(IE) CNCEU2(IE) CNCEU3(IE)	Neutral (1), ionic (2), and adsorbed (3) pollutant concentrations in μg/m^3 in the estuary at points IE downstream and upstream, respectively, of the source.	COMMON/OUT/
CONAQE CONAQL CONAQR CONAQO	Concentration in aquatic organisms in μg/g when estuary, lake, river, and ocean, respectively, is considered.	SUBROUTNE BIOCHN
CONL1 CONL2 CONL3	Neutral, ionic, and adsorbed pollutant concentrations, respectively, in μg/m^3 in the lake.	COMMON/OUT/
CONO1(I) CONO2(I) CONO3(I)	Neutral, ionic, and adsorbed pollutant concentrations, respectively, in μg/m^3 at points I from the source in the ocean.	COMMON/OUT/
CONPLE CONPLL CONPLR CONPLS	Concentration in terrestrial plants (forage) in μg/g when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	SUBROUTINE BIOCHN

CONR1(IR) CONR2(IR) CONR3(IR)	Neutral, ionic, and adsorbed pollutant concentrations, respectively, in $\mu g/m^3$ in reach IR of the river.	COMMON/OUT/
CONSDE CONSDL CONSDO CONSDR	Average suspended sediment concentration in kg/m^3 for estuary, lake, ocean and river, respectively.	COMMON/SDPARE/ COMMON/SDPARL/ COMMON/SDPARO/ COMMON/SDPARR/
COVFLG	Specifies whether the compound is (=YES) or is not (=NO) a covalently bonding material.	SUBROUTINE BIOCHN
CP	Array used to store cubic coefficients c_i (Forsythe, et al., 1977) in spline calculation of trapping efficiency P (Zison, et al., 1977).	SUBROUTINE SEDCON
CTHETA	Array used to store cubic coefficients c_i (Forsythe, et al., 1977) needed in spline calculation of Shields factor (Bagnold, 1966).	SUBROUTINE FUNLAU
CTYLTH	Length of the city or urban area in m when there is an area source.	COMMON/AIRPAR/
CUM	Pollutant concentration in the soil moisture of the upper soil zone in $\mu g/ml$.	SUBROUTINE TRANS3

CUMEST CUMLKE CUMRIV CUMS	Pollutant concentration in the soil moisture of the upper soil zone in μg/ml when estuary, lake river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
CUSA	Pollutant concentration in the soil air of the upper soil zone in μg/ml.	SUBROUTINE TRANS3
CUSAES CUSALK CUSARV CUSAS	Pollutant concentration in the soil air of the upper soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
CVFALL	Array used to store the cubic coefficients c_i (Forsythe, et al., 1977) needed in spline calculation of the fall velocity (Fields, 1976).	SUBROUTINE FUNLAU
DENSDR DENSDT	Density of the sediment in the river and tributary, respectively, in g/cm^3.	COMMON/SDPARR/ COMMON/SDPAPL/
DENWR DENWT	Density of the water in the river and tributary, respectively, in g/cm^3.	COMMON/SDPARR/ COMMON/SDPAPL/
DEPFAC	Depletion factor or term - i.e., the integral used for depleting the source term in point source calculations.	COMMON/CAVPAR/

DFUNC	Array used to store the cubic coefficients d_i (Forsythe, et al., 1977) needed in spline calculation of Laursen's function (Laursen, 1958).	SUBROUTINE FUNLAU
DH	ΔH, the plume rise in m.	SUBROUTINE AIR
DIASDR DIASDT	Median sediment diameter in mm for the river and tributary, respectively.	COMMON/SDPARR/ COMMON/SDPARL/
DIASED	Median sediment diameter in mm.	SUBROUTINE FUNLAU
DIATHE	Array containing values of median sediment diameter in mm that were taken from the Shields factor curve (Bagnold, 1966). See parameter SHIELD below.	SUBROUTINE FUNLAU
DIAVFL	Array containing values of median sediment diameter in mm that were taken from the fall velocity curve (Fields, 1976). See parameter VFL below.	SUBROUTINE FUNLAU
DISFLG	DISFLG = YES if the longitudinal dispersion coefficient for the estuary is known, = NO if not.	COMMON/FLAGS/

DISK	Acid or base dissociation constant in moles/l.	COMMON/EQUIL/
DP	Array used to store the cubic coefficients d_i (Forsythe, et al., 1977) needed in spline calculation of trapping efficiency P for lakes (Zison, et al., 1977).	SUBROUTINE SEDCON
DT	Time step in s.	SUBROUTINES AIR, LEVEL3, and WATER
DTHETA	Array used to store the cubic coefficients d_i (Forsythe, et al., 1977) needed in spline calculation of Shields factor θ (Bagnold, 1966).	SUBROUTINE FUNLAU
DVFALL	Array used to store the cubic coefficients d_i (Forsythe, et al., 1977) needed in spline calculation of the fall velocity (Fields, 1976).	SUBROUTINE FUNLAU
EL	Longitudinal dispersion coefficient in m^2/s for estuary.	COMMON/WPARE/
ENTPY	Enthalpy of the stack gas in j/kg.	COMMON/AIRPAR/
ESTU	ESTU is YES if an estuary is considered, NO if not.	COMMON/FLAGS/

ETA	Evapotranspiration rate in cm/mon.	COMMON/HYR/
F	Array used to store values of Laursen's function taken from Laursen's curve (Laursen, 1958) at points SVFL (see below). This array contains the natural log of the actual points from the curve in order to increase accuracy.	SUBROUTINE FUNLAU
FDEST FDLAKE FDRIV FDSOIL	Dry deposition in kg/m^2/s when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	SUBROUTINE FUNLAU
FGAM	Gamma function at a specified point (Bonazountas and Wagner, 1981).	COMMON/HYR/
FUNC	Function needed in Laursen's formula (Laursen, 1958).	SUBROUTINE FUNLAU
FUNCR FUNCT	Function needed in Laursen's formula (Laursen, 1958) for river and tributary, respectively.	SUBROUTINE SEDCON
FWEST FWLAKE FWRIV FWSOIL	Wet deposition in kg/m^2/s when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	SUBROUTINE AIR

G	Gravitational infiltration parameter (Bonazountas and Wagner, 1981).	COMMON/HYR/
GEOM(1)	GEOM(1) or AR is the surface area in cm^2 of the soil affected by direct pollutant application.	COMMON/AP/
GEOM(2)	Z = GEOM(2)*100.0 is the depth to the groundwater table in cm.	COMMON/AP/
GEOM(3)	GEOM(3) or DU is the depth of the upper unsaturated soil zone in cm.	COMMON/AP/
GEOM(4)	GEOM(4) or DM is the depth of the middle unsaturated soil zone in cm.	COMMON/AP/
GEOM(6)	GEOM(6) or A2KDE is the ratio of the biodegradation rate of the compound in the middle soil zone to the upper soil zone.	COMMON/AP/
GEOM(7)	GEOM(7) or A2OC is the ratio of the organic carbon content of soil in the middle zone to the upper soil zone.	COMMON/AP/

GEOM(8)	GEOM(8) or A2CC is the ratio of the clay content of the soil in the middle soil zone to the upper soil zone.	COMMON/AP/
GEOM(9)	GEOM(9) or AKDE is the ratio of the biodegradation rate of the compound in the lower soil zone to the upper soil zone.	COMMON/AP/
GEOM(10)	GEOM(10) or AOC is the ratio of the organic carbon content of soil in the lower soil zone to the upper soil zone.	COMMON/AP/
GEOM(11)	GEOM(11) or ACC is the ratio of the clay content of the soil in the lower soil zone to the upper soil zone.	COMMON/AP/
GEOM(14)	GEOM(14) or FRN is the Freundlich exponent.	COMMON/AP/
GEOM(15)	GEOM(15) or PH is the pH of the upper soil zone layer.	COMMON/AP/
GEOM(16)	GEOM(16) or A2PH is the ratio of pH for the middle to upper soil layer.	COMMON/AP/
GEOM(17)	GEOM(17) or APH is the ratio of pH for the lower to upper soil layers.	COMMON/AP/

GEOM(18)	GEOM(18) or A2CEC is the ratio of the cation exchange capacity in the middle to upper soil zone.	COMMON/AP/
GEOM(19)	GEOM(19) or ACEC is the ratio of the cation exchange capacity in the lower to upper soil zone.	COMMON/AP/
GRWROF	Groundwater runoff in μg/mon.	SUBROUTINE TRANS3
GZ	Ratio of calculated monthly precipitation to monthly precipitation that was input.	COMMON/HYR/
HEFFIV	Effective stack height in m for point source.	COMMON/CAVPAR/
HMIX(MON,IYR)	Mixing height for month MON and year IYR in m.	COMMON/AIRPAR/
HMIXZ	Same as HMIX(MON,IYR). This parameter is passed via COMMON to FUNCTION´S DEPAVG(X) and CAVGE(X).	COMMON/CAVPAR/
HPLUSE HPLUSL HPLUSO HPLUSR	$[H^+]$ in moles/l when estuary, lake, ocean, and river, respectively, is considered.	COMMON/EQUIL/
HS	Stack height in m.	COMMON/AIRPAR/
HYDBAL(IMO,1)	Soil moisture (THA) as a fraction for month IMO.	COMMON/HB/

HYDBAL(IMO,2)	Precipitation for month IMO in cm (= PA/12).	COMMON/HB/
HYDBAL(IMO,3)	Net infiltration for month IMO in cm (= IA/12).	COMMON/HB/
HYDBAL(IMO,4)	Evapotranspiration for month IMO in cm (= ETA/12).	COMMON/HB/
HYDBAL(IMO,5)	Surface runoff for month IMO in cm (= RSA/12).	COMMON/HB/
HYDBAL(IMO,6)	Groundwater runoff for month IMO in cm (= RGA/12).	COMMON/HB/
HYDBAL(IMO,7)	Yield for month IMO in cm. HYDBAL(IMO,7) = HYDBAL(IMO,6) + HYDBAL(IMO,5).	COMMON/HB/
HYDBAL(IMO,8)	Same as GZ for month IMO.	COMMON/HB/
HYDBAL(IMO,9)	Same as CLIMM2(1,IMO,IYR).	COMMON/HB/
IA	Annual net infiltration in cm.	COMMON/HYR/
IGE	Logical input device number used to read in general climatologic, soil, and chemistry data (is = 1).	COMMON/FI/
IL3	Logical input device number used to read in LEVEL3 data (is = 2).	COMMON/FI/

IMO or IMON	Index signifying month of the year.	Numerous Subroutines
IOR IOW	Logical device number used for reading SESOIL executive data (IOR = 5) and writing SESOIL portion of output (IOW = 6), respectively.	COMMON/FI/
IPASS	Index used to bypass calculation of constant parameters that have already been computed in order to avoid repetition.	SUBROUTINES LEVEL3 and TRANS3
IR	Reach number in the river.	SUBROUTINE OUTPUT
ISTEP	Ten time steps are taken each month and ISTEP is the index used for these steps.	SUBROUTINES AIR, LEVEL3, TRANS3, and WATER
IWATER	IWATER = 1 signifies lake, IWATER = 2 signifies river, and IWATER = 3 signifies estuary. IWATER = 1 and parameter WATBOD=NO signify no water body is considered.	SUBROUTINE LEVEL3 and TRANS3
IYR	IYR is the index for the year.	Numerous Subroutines
IYRS	Index of how many years of data follow.	SUBROUTINE RFILE
JAPPL	Index for application area of interest.	COMMON/EX/

JCH	Index of the chemical compound of interest.	COMMON/EX/
JNUT	Index for the nutrient cycle participation.	COMMON/EX/
JRE	Index of the region of interest.	COMMON/EX/
JRUN	Incremental number of the run.	COMMON/EX/
JSO	Index of the soil type of interest.	COMMON/EX/
JYRS	Number of years to be simulated.	COMMON/EX/
KOW	n-octanol water partition coefficient (dimensionless).	SUBROUTINE BIOCHN
LAKE	LAKE is YES if a lake is considered, NO if not.	COMMON/FLAGS/
LAMBDA	Weathering constant in day^{-1}.	SUBROUTINE BIOCHN
LEVEL	LEVEL = 3, the SESOIL level of operation.	COMMON/EX/
LIGCL	Ligand concentration in the lower soil zone in μg/ml.	SUBROUTINE TRANS3
LIGCLE LIGCLL LIGCLR LIGCLS	Ligand concentration in the lower soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/

LIGCM	Ligand concentration in the middle soil zone in μg/ml.	SUBROUTINE TRANS3
LIGCME LIGCML LIGCMR LIGCMS	Ligand concentration in the middle soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
LIGCU	Ligand concentration in the upper soil zone in μg/ml.	SUBROUTINE TRANS3
LIGCUE LIGCUL LIGCUR LIGCUS	Ligand concentration in the upper soil zone in μg/ml when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
LIGL LIGM LIGU	Ligand mass input to the lower, middle, and upper soil zones, respectively, in μg/cm^2.	COMMON/LEV2/
MON	Index signifying month of the year.	Numerous Subroutines
NCH	Index of the chemical being considered.	SUBROUTINE RFILE
NF	Found in the GE data file input sequence, this index signifies the type of SESOIL data that follow. If NF=1 subsequent data describes the region;	SUBROUTINE RFILE

	if NF=2 subsequent data describes the soil; and if NF=3 subsequent data describes the chemical.	
NPTSE	Number of points on either side of the source at which TOX-SCREEN computes and outputs pollutant concentrations in the estuary.	COMMON/WPARE/
NPTSO	Number of points from pollutant source that TOX-SCREEN computes and outputs pollutant concentrations in the ocean.	COMMON/WPARO/
NR	Number of reaches that the river is broken into.	COMMON/WPARR/
NRE	Index of the site or region being considered.	SUBROUTINE RFILE
NSO	Index of the soil being considered.	SUBROUTINE RFILE
NSTEPS	Number of time steps taken each month (currently = 10).	SUBROUTINES AIR, LEVEL3, TRANS3, and WATER
NTY	Index of the region that the simulation will be applied to.	SUBROUTINE RFILE
OCEAN	OCEAN is YES if an ocean is considered, NO if not.	COMMON/FLAGS/

P	Trapping efficiency for lakes (Zison et al., 1977).	SUBROUTINE SEDCON
PA	Computed annual rainfall in cm.	COMMON/HYR/
PCONC(IMO,15, IWATER)	Array containing pollutant concentrations in soil water, soil air, and adsorbed phases, free ligand concentration, and maximum pollutant depth for month IMO and water body IWATER (see definition of IWATER above).	COMMON/LEV2/
PDAT	Array containing values of trapping efficiency P for lakes taken from curve in Zison et al., 1977. See parameter VDQ below.	SUBROUTINE SEDCON
PI	3.1415927	SUBROUTINE AIR, and FUNCTION CAVGE
PINL PINM PINU	Pollutant mass going to lower, middle, and upper soil zone, respectively, in $\mu g/cm^2$.	SUBROUTINE TRANS3
PMASSE	Pollutant mass in estuary in kg.	SUBROUTINE WATER
POUTL POUTM POUTU	Pollutant mass output from lower, middle, and upper soil zone, respectively, in $\mu g/cm^2$.	SUBROUTINE TRANS3

PREML PREMM PREMU	Pollutant mass remaining at end of time step in lower, middle, and upper soil zone, respectively, in $\mu g/cm^2$.	SUBROUTINE TRANS3
PTHERL PTHERM PTHERU	Pollutant mass available at beginning of time step in lower, middle, and upper soil zone, respectively, in $\mu g/cm^2$.	SUBROUTINE TRANS3
PTRANL PTRANM PTRANU	Pollutant mass transformed within time step in lower, middle, and upper soil zone, respectively, in $\mu g/cm^2$.	SUBROUTINE TRANS3
QH	Heat emission term due to gas efflux used in plume rise equations (j/s).	SUBROUTINE AIR
QP	Depleted source term in kg/s.	SUBROUTINE AIR
QS(MON,IYR)	Pollutant source rate to air for month MON and year IYR in kg/s.	COMMON/AIRPAR/
R	Initial interception fraction.	SUBROUTINE BIOCHN
RATIO	Parameter needed in Laursen's formula to compute sediment concentration. RATIO is the ratio of the sediment diameter to water depth raised to the 7/6 power.	SUBROUTINE FUNLAU

RATIOR RATIOT	Same as RATIO for river and tributary, respectively.	SUBROUTINE SEDCON
RESUSE RESUSL RESUSR RESUSS	Pollutant concentration in air due to resuspension from soil in μg/m^3 when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
RGA	Computed annual groundwater runoff in cm.	COMMON/HYR/
RHO	Stack gas density in kg/m^3.	COMMON/AIRPAR/
RIVER	RIVER is YES if a river is considered, NO if not.	COMMON/FLAGS/
RSA	Computed annual surface runoff in cm.	COMMON/HYR/
RUNM1(1,MON) RUNM1(2,MON) RUNM1(3,MON)	Also called CUM, CMM, and CLM, respectively; these input parameters (if nonzero) are the concentrations of the pollutant in the soil moisture of the upper, middle, and lower soil zones in month MON (μg/ml).	COMMON/AP/
RUNM1(4,MON) RUNM1(5,MON) RUNM1(6,MON)	Also called POLINU, POLINM, and POLINL, respectively; these input parameters are the monthly pollution load in μg/cm^2 entering the upper, middle, and	COMMON/AP/

	lower soil zones (i.e., there is a direct application).	
RUNM1(7,MON)	Also called ISRM, this is the monthly index for pollutant appearance in surface runoff. ISRM is a number between 0.0 and 1.0 with 0.0 signifying no surface runoff is allowed.	COMMON/AP/
RUNM2(1,MON)	Also called ASL, this is the monthly ratio of the concentration of pollutant in rain to the maximum solubility in water. This SESOIL parameter is not used in TOX-SCREEN.	COMMON/AP/
RUNM2(2,MON) RUNM2(3,MON) RUNM2(4,MON)	Also called TRANSU, TRANSM, and TRANSL, respectively, these input parameters represent the monthly amount of pollutant transformed ($\mu g/cm^2$) in the upper, middle, and lower soil zones, and not accounted for by existing model processes.	COMMON/AP/
RUNM2(5,MON) RUNM2(6,MON) RUNM2(7,MON)	Also called SINKU, SINKM, and SINKL, respectively, these input parameters represent the monthly amount of pollutant "lost" ($\mu g/cm^2$) in the upper, middle, and lower soil zone, by processes not directly described by the model (e.g., plant uptake).	COMMON/AP/

RUNM2(8,MON) RUNM2(9,MON) RUNM2(10,MON)	Also called LIGU, LIGM, and LIGL, respectively, these parameters are the monthly ligand mass input to the upper, middle, and lower soil zones in μg/cm^2.	COMMON/AP/
SACON	Concentration in air in kg/m^3 due to volatilization of pollutant from soil.	SUBROUTINE AIR
SAMIN	Volatilization rate in kg/s from soil to air.	SUBROUTINE AIR
SAMOUE SAMOUL SAMOUR SAMOUS	Soil to air volatilization rate in kg/sec when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
SAMOUT	Soil to air volatilization rate in μg/mon.	SUBROUTINE TRANS3
SCONLE SCONLL SCONLR SCONLS	Pollutant concentration in μg/m^3 in the lower soil zone when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
SCONME SCONML SCONMR SCONMS	Pollutant concentration in μg/m^3 in the middle soil zone when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
SCONUE SCONUL	Pollutant concentration in μg/m^3 in the upper soil zone when estuary,	COMMON/OUT/

SCONUR SCONUS	lake, river, and soil (i.e., no water body) option, respectively, is considered.	
SEDCE(MON,IYR) SEDCL(MON,IYR) SEDCO(MON,IYR) SEDCR(MON,IYR)	Average suspended sediment concentration in kg/m^3 for month MON and year IYR when estuary, lake, ocean, and river option, respectively, is considered. (If flag SEDLKE is NO and flag TRICON is YES, then SEDCL(MON,IYR) is the sediment concentration in the tributary flowing into the lake.)	COMMON/SDPARE/ COMMON/SDPARL/ COMMON/SDPARO/ COMMON/SDPARR/
SEDLKE	SEDLKE is YES if the suspended sediment concentration in the lake is known, NO if not.	COMMON/FLAGS/
SEDRIV	SEDRIV is YES if the suspended sediment concentration in the river is known, NO if not.	COMMON/FLAGS/
SHEAR	Used in Laursen's formula for sediment concentration, SHEAR is the square root of the boundary shear.	SUBROUTINE FUNLAU
SHIELD	Array containing values of Shields factor at different sediment diameters (see parameter DIATHE above) from the curve given in Bagnold, 1966.	SUBROUTINE FUNLAU
SIGMA	Capillary infiltration parameter.	COMMON/HYR/

SIGMAY	Horizontal dispersion coefficient σ_y in m.	SUBROUTINE AIR and FUNCTION CAVGE
SIGMAZ	Vertical dispersion coefficient σ_z in m.	SUBROUTINE AIR and FUNCTIONS CAVGE and DEPAVG
SIGZMX	Limiting value of SIGMAZ or maximum SIGMAZ allowed.	SUBROUTINE AIR and FUNCTIONS CAVGE and DEPAVG
SLAREA	Sum of lake area and soil area next to lake affected by pollutant contamination (m^2).	SUBROUTINE AIR
SLM	Concentration of pollutant on soil solids in μg/g soil for the lower soil zone.	SUBROUTINE TRANS3
SLMEST SLMLKE SLMRIV SLMS	Concentration of pollutant on soil solids in μg/g soil for the lower soil zone when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
SLOPER SLOPET	Slope of the river and tributary to lake, respectively.	COMMON/SDPARR/ COMMON/SDPART/

SMM	Concentration of pollutant on soil solids in µg/g soil for the middle soil zone.	SUBROUTINE TRANS3
SMMEST SMMLKE SMMRIV SMMS	Concentration of pollutant on soil solids in µg/g soil for the middle soil zone when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
SOIL1(1)	SOIL1(1) or RS is the soil density in g/cm^3.	COMMON/SO/
SOIL1(2)	SOIL1(2) or K1 is the soil intrinsic permeability in cm^2.	COMMON/SO/
SOIL1(3)	SOIL1(3) or C is the soil disconnectedness index and is dimensionless.	COMMON/SO/
SOIL1(4)	SOIL1(4) or N is the effective soil porosity and is dimensionless.	COMMON/SO/
SOIL1(5)	SOIL1(5) or OC is the organic content of the soil in % oc.	COMMON/SO/
SOIL1(6)	SOIL1(6) or CC is the clay content of the soil in % cc.	COMMON/SO/
SOIL2(1)	SOIL2(1) or CEC is the soil exchange capacity in meq/100 g soil.	COMMON/SO/

SOIL2(2) SOIL2(3) SOIL2(4)	Also called K1U, K1M, and K1L, respectively; these parameters are the intrinsic permeability in cm^2 of the upper, middle, and lower soil zones.	COMMON/SO/
SOIL2(5)	SOIL2(5) or RDUST is the dust loading factor in μg soil/m^3.	COMMON/SO/
SRAD	The stack radius in m when there is a point source.	COMMON/AIRPAR/
SUM	Concentration of pollutant on soil solids in μg/g soil for the upper soil zone.	SUBROUTINE TRANS3
SUMEST SUMLKE SUMRIV SUMS	Concentration of pollutant on soil solids in μg/g soil for the upper soil zone when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/MEDIA/
SURROF	Pollutant in surface runoff in μg/mon.	SUBROUTINE TRANS3
SVFL	Array used to store values of $\sqrt{\tau_0/\rho}$ /w from Laursen's curve (Laursen, 1958). See parameter F above. This array contains the natural log of the actual points from the curve in order to increase accuracy.	SUBROUTINE FUNLAU
SVOLAE SVOLAL	Volatilization rate in μg/mon from soil to air when estuary,	COMMON/OUT/

SVOLAR SVOLAS	lake, river, and soil (i.e., no water body) option, respectively, is considered.	
SWGRWE SWGRWL SWGRWR SWGRWS	Polluted groundwater runoff rate in µg/mon when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/
SWKSW	Soil-water partition coefficient in moles/kg/moles/l.	COMMON/EQUIL/
SWMINE SWMINL SWMINR	Soil to water pollutant rate in kg/s at beginning of time step. This is the sum of surface and groundwater pollutant runoff when estuary, lake, and river option, respectively, is considered.	COMMON/MEDIA/
SWMOUE SWMOUL SWMOUR	Soil to water pollutant rate in kg/s computed at end of time step. This is the sum of surface and groundwater pollutant runoff when estuary, lake, and river option, respectively, is considered.	COMMON/MEDIA/
SWSURE SWSURL SWSURR SWSURS	Pollutant in surface runoff from soil to water in µg/mon when estuary, lake, river, and soil option, respectively, is considered.	COMMON/OUT/
TCRIT	Critical tractive force for beginning of sediment transport in kg/m^2.	SUBROUTINE FUNLAU

TCRITR TCRITT	TCRIT for river and tributary (flowing into lake), respectively.	SUBROUTINE SEDCON
TE	Growth period before harvest in days.	SUBROUTINE BIOCHN
THA	Soil moisture content (fraction).	COMMON/HYR/
THETA	Shields factor used in calculation of TCRIT (Laursen, 1958 and Bagnold, 1966).	SUBROUTINE FUNLAU
THM	Soil moisture content (fraction) at beginning of time step.	COMMON/LEV2)
TIDMAX	Maximum tidal velocity in m/s.	COMMON/WPARE/
TITLE(12)	Array that holds headings for various sections of the SESOIL GE data file.	SUBROUTINE RFILE
TITLES(1,12)	Heading or title of the area or region where model will be applied.	COMMON/TI/
TITLES(2,12)	Heading or title used to describe the soil type.	COMMON/TI/
TITLES(3,12)	Heading or title used to describe the chemical.	COMMON/TI/
TITLES(4,12)	Heading or title used to describe the nutrient data (not used at present).	COMMON/TI/

TITLES(5,12)	Heading or title used to describe the region/application.	COMMON/TI/
TOPRIM	Boundary shear τ_0' associated with sediment particles (kg/m^2).	SUBROUTINE SEDCON
TRICON	Used only when flag LAKE is YES and flag SEDLKE is NO; TRICON is YES if the suspended sediment concentration of a tributary flowing into the lake is known, NO if not.	COMMON/FLAGS/
U	Wind speed in m/s.	COMMON/CAVPAR/
UDG UDP	Dry deposition velocity for gases and particulates, respectively.	COMMON/AIRPAR/
UDPW	Sum of dry and wet deposition velocities.	COMMON/CAVPAR/
UW(MON,IYR)	Wind speed for month MON and year IYR in m/s.	COMMON/AIRPAR/
UWET	Wet deposition velocity in m/s.	SUBROUTINE AIR
UWG	Wet deposition velocity for gases in m/s.	SUBROUTINE AIR
VDQ	Array containing points (volume divided by flow rate) at which the trapping efficiency P for lakes were taken from curve given in Zison et al., 1977. See parameter PDAT above.	SUBROUTINE SEDCON

VFALL	Sediment fall velocity in m/s used in Laursen's formula to compute sediment concentration.	SUBROUTINE FUNLAU
VFL	Array containing sediment fall velocity values in m/s taken from velocity curve given in Fields, 1976. See parameter DIAVFL above.	SUBROUTINE FUNLAU
VG	Gravitational settling velocity of the pollutant in m/s.	COMMON/CAVPAR/
VOLFLO	Volume of lake divided by the flow rate out of lake in s.	SUBROUTINE SEDCON
VS	Stack gas exit velocity in m/s.	COMMON/AIRPAR/
WAMOUE WAMOUL WAMOUR(IR)	Volatilization rate in kg/sec from water to air when estuary, lake, and river (reach IR) option, respectively, is considered.	COMMON/MEDIA/
WASHE WASHL WASHR WASHS	Surface washload (erosion by water) in μg/mon when estuary, lake, river, and soil (i.e., no water body) option, respectively, is considered.	COMMON/OUT/

WATBOD	WATBOD is YES if any water body (i.e., estuary, lake, ocean, or river) is considered in a simulation, NO if not.	COMMON/FLAGS/
WCINO(MON,IYR)	0.02 times the concentration of the effluent to the ocean for month MON and year IYR (kg/m^3).	COMMON/WPARO/
WDEPE WDEPL WDEPR WDEPT	Average water depth of estuary, lake, river, and tributary (flowing into lake), respectively, in m.	COMMON/WPARE/ COMMON/WPARL/ COMMON/WPARR/ COMMON/SDPARL/
WKB? WKH? WKO? WKP? WKV?	Rate constants in water in s^{-1} for biodegradation, hydrolysis, oxidation, photolysis, and volatilization, respectively. ? is E for estuary, L for lake, O for ocean, and R for river.	COMMON/WRATES/
WKDL WKDR	Rate at which water flows out of lake and river, respectively, in s^{-1}.	SUBROUTINE WATER
WKTOT?	Sum of WKB?, WKH?, WKO?, WKP?, and WKV? where ? is E for estuary, L for lake, O for ocean, and R for river.	SUBROUTINE WATER
WLENE WLENR	Length of estuary and each river reach, respectively, in m.	COMMON/WPARE/ COMMON/WPARR/

WMINE(MON,IYR) WMINL(MON,IYR) WMINR(MON,IYR)	Pollutant source rate into estuary, lake, and river, respectively, in kg/s for month MON and year IYR.	COMMON/WPARE/ COMMON/WPARL/ COMMON/WPARR/
WMTLKE WMTRIV(IR)	Mass of pollutant in lake and river reach IR, respectively, in kg.	COMMON/WPARL/ COMMON/WPARR/
WMTOLD	Mass of pollutant in kg in a river reach from the previous time step.	COMMON/WPARR/
WRATG WRATP	Washout ratio for gases and particulates, respectively.	COMMON/AIRPAR/
WSACON	Concentration in air in kg/m^3 due to volatilization from both water and soil.	SUBROUTINE AIR
WSAMIN	Volatilization rate from water and soil to air in kg/s.	SUBROUTINE AIR
WVELE(MON,IYR) WVELL(MON,IYR) WVELO(MON,IYR) WVELR(MON,IYR)	Current velocity in m/s for month MON and year IYR when estuary, lake, ocean, and river option, respectively, is considered.	COMMON/WPARE/ COMMON/WPARL/ COMMON/WPARO/ COMMON/WPARR/
WVOLAE WVOLAL	Volatilization rate from water in μg/mon when estuary, lake,	COMMON/OUT/

WVOLAR	and river option, respectively, is considered.	
WVOLE WVOLL WVOLR	Water volume in m^3 when estuary, lake, and river option, respectively, is considered.	SUBROUTINE WATER COMMON/WPARL/ COMMON/WPARR/
WWIDE WWIDR	Average width in m when estuary and river option, respectively, is considered.	COMMON/WPARE/ COMMON/WPARR/
XESTY(I)	Array that contains the distances both up- and downstream from the center of the estuary in which concentrations are computed when the estuary option is considered.	COMMON/OUT/
XI	Surface runoff function (Bonazountas and Wagner, 1981).	COMMON/HYR/
XLENS	When no water body is considered, and there is a point source, XLENS is the length of the plume considered over the soil in m.	COMMON/SPARS/
XMAX	Distance to point of maximum centerline concentration in m when there is a point source.	COMMON/CAVPAR/

XOCEAN	Distance in m between points in the ocean at which TOX-SCREEN computes and outputs pollutant concentrations.	COMMON/WPARO/
XSOIL	Distance in m to the far edge of the watershed from the lake when there is a point source.	COMMON/SPARL/
YA	Computed annual surface and groundwater runoff in cm.	COMMON/HYR/
YV	Terrestrial plant productivity in g/m^2.	SUBROUTINE BIOCHN

APPENDIX A
REFERENCES

1. Bagnold, R. A., An Approach to the Sediment Transport Problem from General Physics, Geological Survey Professional Paper 422-I, U.S. Government Printing Office (1966).

2. Bonazountas, M. and J. Wagner, SESOIL: A Seasonal Soil Compartment Model, Draft Report, Arthur D. Little, Inc., Cambridge, Mass., Prepared for the U.S. Environmental Protection Agency, Office of Toxic Substances (1981).

3. Fields, D. E., CHNSED: Simulation of Sediment and Trace Contaminant Transport with Sediment/Contaminant Interaction, ORNL/NSF/EATC-19, Oak Ridge National Laboratory (1976).

4. Forsythe, G. E., M. A. Malcolm, and C. B. Moler, Computer Methods for Mathematical Computations, Prentice-Hall, Inc. (1977).

5. Laursen, E. M., "The Total Sediment Load of Streams," Paper #1530 in Proceedings of ASCE 84, HY1 (1958).

6. McDowell-Boyer, L. M. and D. M. Hetrick, A Multimedia Screening-Level Model for Assessing the Potential Fate of Chemicals Released to the Environment, ORNL/TM-8334, Oak Ridge National Laboratory (1982).

7. Zison, S. W., K. F. Haven, and W. B. Mills, Water Quality Assessment: A Screening Method for Nondesignated 208 Areas, EPA-600/9-77-023, U.S. Environmental Protection Agency, Office of Research and Development (1977).

APPENDIX B

JOB CONTROL LANGUAGE TO RUN TOX-SCREEN ON IBM 3033 COMPUTER

```
//UIDSCTOX JOB (#####,IO2),'NAME AND ADDRESS',TIME=(,40)
/*ROUTE  PRINT LOCAL
/*JOBPARM LINES=20
// EXEC FORTHCLG,PARM.FORT='XREF',PARM.GO='EU=-1,DUMP=I',REGION.GO=150K
//*  TOX-SCREEN FORTRAN FOLLOWS
//FORT.SYSIN DD *
=SCREEN.TOX
/*
//*  NEXT OUTPUT FILE CONTAINS INPUT DATA AND ERROR MESSAGES
//GO.FT13F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
//*  NEXT OUTPUT FILE CONTAINS LAKE RESULTS OR SOIL-AIR
//*  INTERACTION RESULTS
//GO.FT14F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
//* NEXT OUTPUT FILE CONTAINS RIVER RESULTS
//GO.FT15F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
//*  NEXT OUTPUT FILE CONTAINS ESTUARY RESULTS
//GO.FT16F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
//*  NEXT OUTPUT FILE CONTAINS OCEAN RESULTS
//GO.FT17F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
//*  NEXT OUTPUT FILE CONTAINS RESULTS FROM FOOD CHAIN BIOACCUMULATION
//GO.FT19F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
//*  NEXT OUTPUT FILE CONTAINS RESULTS FROM SESOIL PORTION OF TOX-SCREEN
//GO.FT06F001 DD SYSOUT=A,DCB=(RECFM=VBA,LRECL=137,BLKSIZE=1100)
/*
//*  NEXT INPUT FILE CONTAINS SESOIL GE DATA
//GO.FT01F001 DD *
=FOR01.DAT
//*  NEXT INPUT FILE CONTAINS SESOIL L3 DATA
//GO.FT02F001 DD *
=FOR02.DAT
//*  NEXT INPUT FILE CONTAINS SESOIL EXEC DATA
//GO.FT05F001 DD *
=FOR05.DAT
//*  NEXT INPUT FILE CONTAINS MODEL FLAG PARAMETERS
//GO.FT10F001 DD *
=FOR10.DAT
//*  NEXT INPUT FILE CONTAINS AIR COMPARTMENT PARAMETERS
//GO.FT11F001 DD *
=FOR11.DAT
//*  NEXT INPUT FILE CONTAINS WATER COMPARTMENT PARAMETERS
//GO.FT12F001 DD *
=FOR12.DAT
//*  NEXT INPUT FILE CONTAINS BIOACCUMULATION PARAMETERS
//GO.FT18F001 DD *
=FOR18.DAT
/*
//
ENDINPUT
```

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APPENDIX C
SAMPLE INPUT DATA

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FOR05.DAT

```
    1    3    1    1    1    0    1    1
  999
```

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FOR01.DAT

```
1      REGIONAL DESCRIPTIONS; CLIMATIC,STORM DATA: (TEST DATA ONLY)
     1 CLINTON,MASS.(40 YR AVERAGED DATA FOR TEST ONLY)     1
 L       39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00 39.00
 TA       14.3  14.3  14.3  14.3  14.3  14.3  14.3  14.3  14.3  14.3  14.3  14.3
 MN        .30   .30   .30   .30   .30   .30   .30   .30   .30   .30   .30   .30
 S         .60   .60   .60   .60   .60   .60   .60   .60   .60   .60   .60   .60
 A        0.1   0.1   0.1   0.1   0.1   0.1   0.1   0.1   0.1   0.1   0.1   0.1
 REP      0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
 MPM     10.54  4.57  0.13  3.40  2.31 10.54  2.62 12.32  1.42  2.21 14.88  3.02
 MTR       .18   .18   .18   .18   .18   .18   .18   .18   .18   .18   .18   .18
 MN       13.0  6.00  1.00  4.00  3.00  13.0  4.00  14.0  2.00  3.00  17.0  4.00
 MT      30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42 30.42

2      SOIL CLASSIFICATION DATA: (TEST DATA ONLY)
     1 SILTY-LOAM-KANSAS
         - RS,K1,C,N,OC,CC                 1.32 7.E-09   6.00   0.35    15.
         - CEC,K1U,K1M,K1L,RDUST           0.00
3      CHEMISTRY DATA;   (TEST DATA ONLY)
     1 TRICHLOROETHYLENE(TCE)
       SL,KOC,DA,KDE,H,K                1100.00 100.00  .0830   0.009.44E-3   0.00
       MWT,VAL,KNH,KBH,KAH                 0.00   0.00   0.00   0.00   0.00   0.00
       SK,B,MWTLIG                         0.00   0.00   0.00   0.00   0.00   0.00
9      END FILE
```

FOR02.DAT

```
    1 TEST RUN                                              1
        -AR,S,DU,DN,FRN                   0.00   50.00   15.00    10.0    1.40
        -PH,A2PH,APH                      8.00    1.00    .875
        -A2KDE,AKDE,A2OC,AOC,A2CC,ACC     1.10    1.10    1.20    1.20    1.30    1.30
        -A2CEC,ACEC                       1.30    1.30
  CUM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  CMM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  CLM       0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  POLINU    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  POLINM    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  POLINL     0.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  ISRM      1.00  1.00  1.00  1.00  1.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  ASL       .00   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  TRANSU    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  TRANSM    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  TRANSL    0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  SINKU     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  SINKM     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  SINKL     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  LIGCU     00.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  LIGCM     0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
  LIGCL     00.0  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.0
9      END OF FILE
```

FOR10.DAT

```
POINT      GAS                  AIRFLG, AIRPOL
 YES        NO        NO        LAKE, SEDLKE, TRICON
 YES        NO                  RIVER, SEDRIV
 YES       YES                  ESTU, DISFLG
 YES                            OCEAN
ACID                            CHMFLG
```

FOR11.DAT

```
UW(MON,IYR),MON=1,6        5.0      5.0      5.0      5.0      5.0      5.0
            MON=7,12       5.0      5.0      5.0      5.0      5.0      5.0
UDG,WRATG,AK             0.010     2.27   1.6E-5
QS(MON,IYR),MON=1,6     2.2E-3   2.2E-3   2.2E-3   2.2E-3   2.2E-3   2.2E-3
            MON=7,12    2.2E-3   2.2E-3   2.2E-3   2.2E-3   2.2E-3   2.2E-3
HMIX(MN,IYR),MN=1,6     2000.0   2000.0   2000.0   2000.0   2000.0   2000.0
             MN=7,12    2000.0   2000.0   2000.0   2000.0   2000.0   2000.0
HS,VG,VS,SRAD,RHO,EM      100.    0.000      0.0      10.     0.66   2.50E5
```

FOR12.DAT

```
DISK                       0.0
WMINL(MN,IY),MN=1,6       0.01      0.01      0.01      0.01      0.01      0.01
             MN=7,12      0.01      0.01      0.01      0.01      0.01      0.01
WVELL(MN,IY),MN=1,6        0.5       0.5       0.5       0.5       0.5       0.5
             MN=7,12       0.5       0.5       0.5       0.5       0.5       0.5
AREAL,WDEPL,XSOIL,H+ 3.750E+06       2.0     500.0   1.00E-7
WKP,H,O,B,V,SWKSWL   6.200E-08       0.0       0.0       0.0   5.56E-5       15.
SEDIMENT PARAMETERS       0.45      2.65       1.0      2.00     .0001
WMINR(MN,IY),MN=1,6       0.01      0.01      0.01      0.01      0.01      0.01
             MN=7,12      0.01      0.01      0.01      0.01      0.01      0.01
WVELR(MN,IY),MN=1,6        1.5       1.5       1.5       1.5       1.5       1.5
             MN=7,12       1.5       1.5       1.5       1.5       1.5       1.5
NR                           3
WLENR,WWIDR,WDEPR,H+      500.      300.       10.    1.0E-7
WKP,H,O,B,V,SWKSWR   6.200E-08       0.0       0.0       0.0   5.56E-5       15.
SEDIMENT PARAMETERS        .45      2.65       1.0    7.5E-5
WMINE(MN,IY),MN=1,6       0.01      0.01      0.01      0.01      0.01      0.01
             MN=7,12      0.01      0.01      0.01      0.01      0.01      0.01
WVELE(MN,IY),MN=1,6        0.5       0.5       0.5       0.5       0.5       0.5
             MN=7,12       0.5       0.5       0.5       0.5       0.5       0.5
NPTSE                        2
ESTUARY PARAMETERS     25000.0     150.0       2.0      75.0              1.0E-7
WKP,H,O,B,V,SWKSWE   6.200E-08       0.0       0.0       0.0   5.56E-5       15.
SEDCE(MN,IY),MN=1,6      0.025     0.025     0.025     0.025     0.025     0.025
             MN=7,12     0.025     0.025     0.025     0.025     0.025     0.025
WCINO(MN,IY),MN=1,6       0.01      0.01      0.01      0.01      0.01      0.01
             MN=7,12      0.01      0.01      0.01      0.01      0.01      0.01
WVELO(MN,IY),MN=1,6        0.5       0.5       0.5       0.5       0.5       0.5
             MN=7,12       0.5       0.5       0.5       0.5       0.5       0.5
BO,XOCEAN,H+               5.0      500.    1.0E-7
WKP,H,O,B,V,SWKSWO   6.200E-08       0.0       0.0       0.0   5.56E-5       15.
NPTSO                        3
SEDCO(MN,IY),MN=1,6      0.025     0.025     0.025     0.025     0.025     0.025
             MN=7,12     0.025     0.025     0.025     0.025     0.025     0.025
```

FOR18.DAT

```
  NO        COVFLG
 KOW,R,YV,LAMBDA,TE    1.000E+02 4.000E-01 1.500E+02 2.500E-02 3.000E+01
```

APPENDIX D

SAMPLE OUTPUT FORMAT

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To save space in this appendix, only the results for first month (October) and last month (September) are given from files FOR14.DAT, FOR15.DAT, FOR16.DAT, and FOR17.DAT.

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FOR06.DAT

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********************************************************************************

RUN :  1              ****** LEVEL3 SESOIL MODEL OPERATION ******
                       MONTHLY SITE SPECIFIC SIMULATION(3 LAYERS)


    **************************************************************************************************
    *****                                                                                       *****
    ***** SESOIL-82:   SEASONAL CYCLES OF WATER, SEDIMENT, AND POLLUTANTS IN SOIL ENVIRONMENTS   *****
    *****                                                                                       *****
    ***** DEVELOPERS:  M. BONAZOUNTAS,ARTHUR D. LITTLE INC.  ,(617)864-5770,X5871                *****
    *****              J. WAGNER     ,ARTHUR D. LITTLE INC.  ,(617)864-5770,X2505                *****
    *****                                                                                       *****
    ***** VERSION:     JULY 1982                                                                *****
    *****                                                                                       *****
    *****                                                                                       *****
    **************************************************************************************************

                 INDEX
         REGION    : (    1)     CLINTON,MASS.(40 YR AVERAGED DATA FOR TEST ONLY)
         SOIL TYPE : (    1)     SILTY-LOAM-KANSAS
         COMPOUND  : (    1)     TRICHLOROETHYLENE(TCE)
         APPL. AREA: (    1)     TEST RUN

         GENERAL INPUT PARAMETERS
         ========================


     -- APPLICATION PARAMETERS --

AREA(SQ.CM): .00E+00
DEPTH TO GRW(M): 50.
UPPER SOIL ZONE DEPTH(CM): 15.
MIDDLE SOIL ZONE DEPTH(CM): 10.
FREUNDLICH EXPONENT(-): 1.4
PH UPPER ZONE(-): 8.0
PH RATIO MIDDLE:UPPER ZONE(-): 1.0
PH RATIO LOWER:UPPER ZONE(-): .80
DEGRADATION RATIO MIDDLE:UPPER ZONE(-): 1.1
DEGRADATION RATIO LOWER:UPPER ZONE(-): 1.1
ORGANIC CARBON CONTENT RATIO MIDDLE:UPPER ZONE(-): 1.2
ORGANIC CARBON CONTENT RATIO LOWER:UPPER ZONE(-):1.2
CLAY CONTENT RATIO MIDDLE:UPPER ZONE(-): 1.3
CLAY CONTENT RATIO LOWER:UPPER ZONE(-): 1.3
CATION EXCHANGE CAPACITY RATIO MIDDLE:LOWER ZONE(-): 1.3
CATION EXCHANGE CAPACITY RATIO LOWER:UPPER ZONE(-): 1.3


     -- CHEMICAL PARAMETERS --
```

```
SOLUBILITY(UG/ML): .11E+00
ADSORP. COEF.(KOC): .10E+03
DIF. COEF. IN AIR(SQ.CM/SEC): .63E-01
DEGRADATION RATE(/DAY): .00E+00
HENRYS CON.(CU.M-ATM/MOLE):.99E-03
ADSORP. COEF. ON SOIL(K): .00E+00
MOLECULAR  WT.(G/MOL): .00E+00
VALENCE(-): .00E+00
NEUTRAL HYDROLYSIS CONSTANT(/DAY): .00E+00
BASE HYDROLYSIS CONSTANT(L/MOL-DAY): .00E+00
ACID HYDROLYSIS CONSTANT(L/MOL-DAY): .00E+00
LIGAND-POLLUTANT STABILITY CONST.(-): .00E+00
NO. MOLES LIGAND/MOLE POLLUTANT(-): .00E+00
LIGAND MOLECULAR WEIGHT(G/MOL): .00E+00


    -- SOIL PARAMETERS --

DENSITY(G/CU.CM): 1.3
INT. PERMEABILITY(SQ.CM): .70E-08
DISCONNECTEDNESS INDEX(-): 6.0
POROSITY(-): .35
ORGANIC CARBON CONTENT(%): 15.
CLAY CARBON CONTENT(%): .00E+00
CATION EXCHANGE CAPY. (MILLI EQ./1000 DRY SOIL): .00E+00
INTRINSIC PERMEABILITY-UPPER ZONE(SQ.CM): .00E+00
INTRINSIC PERMEABILITY-MIDDLE ZONE(SQ.CM): .00E+00
INTRINSIC PERMEABILITY-LOWER ZONE(SQ.CM): .00E+00
DUST LOADING FACTOR (UG(SOIL)/M**3): .00E+00



                    YEAR- 1  MONTHLY INPUT PARAMETERS
                    -------  ------------------------

                     OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP


    -- CLIMATIC PARAMETERS --

LATITUDE(DEG)        39.0     39.0     39.0     39.0     39.0     39.0     39.0     39.0     39.0     39.0     39.0     39.0
TEMP.(DEG C)         14.3     14.3     14.3     14.3     14.3     14.3     14.3     14.3     14.3     14.3     14.3     14.3
CLOUD CVR(FRAC.)     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300     .300
REL. HUMID.(FRAC.)   .600     .600     .600     .600     .600     .600     .600     .600     .600     .600     .600     .600
ALBEDO(-)          .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00 .100E+00
EVAPOT.(CM/DAY)    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

PRECIP.(CM)          10.5     4.57     .130     3.40     3.31     10.5     2.42     12.3     1.02     2.21     14.9     3.02
M.TIME RAIN(DAYS)    .100     .100     .100     .100     .100     .100     .100     .100     .100     .100     .100     .100
M. STORM NO.(-)      13.0     6.00     1.00     8.00     3.00     13.0     4.00     14.0     2.00     3.00     17.0     6.00
M. SEASON(DAYS)      30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4     30.4



    -- RUN DATA-SET 1 --

MOIS. CONC-UP.(UG/ML) .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
MOIS. CONC-MI.(UG/ML) .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
MOIS. CONC-LO.(UG/ML) .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
POL. INP-U(UG/SQ.CM)  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
POL. INP-M(UG/SQ.CM)  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
POL. INP-L(UG/SQ.CM)  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SUR. RUNOFF(1-Y,0-N)  1.00     1.00     1.00     1.00     1.00   .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

    -- RUN DATA-SET 2 --

CONC. IN RAIN(UG/ML)  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
TRNSFORMED-U(UG/SQ.CM).000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
TRNSFORMED-M(UG/SQ.CM).000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
TRNSFORMED-L(UG/SQ.CM).000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SINKS-U(UG/SQ.CM)     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SINKS-M(UG/SQ.CM)     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SINKS-L(UG/SQ.CM)     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
LIG.INPUT-U(UG/SQ.CM) .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
LIG.INPUT-M(UG/SQ.CM) .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
LIG.INPUT-L(UG/SQ.CM) .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
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                    YEAR - 1  MONTHLY RESULTS (OUTPUT)
                    --------  ------------------------



        -- HYDROLOGIC CYCLE COMPONENTS --


                      OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

SOIL MOISTURE( %)   11.0      10.7      10.1      9.92      9.64      10.5      10.1      11.2      10.5      10.1      11.6      11.0
PRECIPATION(CM)     10.5      4.66      .191      3.53      2.38      10.5      2.72      12.3      1.46      2.36      14.8      3.10
NET INFILTR.(CM)    10.5      4.66      .191      3.53      2.38      10.5      2.72      12.3      1.46      2.36      14.8      3.10
EVAPOTRANSP.(CM)    6.19      4.02      3.02      3.54      2.94      5.86      3.67      6.34      3.05,     3.29      6.65      4.39
SURFACE RUNOFF(CM) .161E-03  .372E-04  .274E-24  .753E-04  .187E-04  .153E-03  .306E-05  .414E-03  .546E-05  .124E-04  .497E-03  .234E-04
GRW RUNOFF(CM)      1.37      1.15      .798      .719      .603      1.02      .798      1.47      1.04      .815      1.07      1.34
YIELD (CM)          1.37      1.15      .798      .719      .603      1.02      .798      1.47      1.04      .815      1.07      1.34




RATIO PA/MPA(GE)    .993      1.02      1.07      1.04      1.03      .999      1.04      1.00      1.03      1.07      .994      1.03
   -------------------------------------------------------

   WATER BODY IS A LAKE

   CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 =  5.625E+05

   -------------------------------------------------------



     -- POLLUTANT MASS INPUT TO COLUMN(UG) --


                      OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

PRECIPATION         .133E+07 .935E+06 .115E+06 .579E+06 .452E+06 .176E+07 .635E+06 .206E+07 .462E+06 .412E+06 .205E+07 .774E+06
OTHER(UPPER)        .145E+12 .204E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .206E+12 .207E+12
OTHER(MIDDLE)       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER(LOWER)        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00


TOTAL INPUT         .145E+12 .204E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .207E+12 .206E+12 .207E+12
     -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) --

   UPPER SOIL ZONE:

SURFACE RUNOFF      .724E+04 .646E+04 .595E-16 .167E+05 .406E+04 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
VOLATILIZED         .360E+11 .145E+12 .198E+12 .207E+12 .210E+12 .193E+12 .209E+12 .191E+12 .211E+12 .214E+12 .186E+12 .209E+12
OTHER SINKS         .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL        .100E+12 .166E+12 .174E+12 .174E+12 .176E+12 .188E+12 .177E+12 .190E+12 .186E+12 .179E+12 .196E+12 .194E+12
IMMOBILIZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED            .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-MOI      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.      .189E+09 .334E+09 .337E+09 .329E+09 .311E+09 .366E+09 .345E+09 .421E+09 .385E+09 .352E+09 .459E+09 .426E+09
IN SOIL AIR         .164E+09 .303E+09 .333E+09 .334E+09 .320E+09 .341E+09 .341E+09 .359E+09 .358E+09 .346E+09 .369E+09 .372E+09

   MIDDLE SOIL ZONE:

VOLATILIZED         .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER SINKS         .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL        .293E+09 .789E+09 .693E+09 .114E+10 .114E+10 .346E+10 .346E+10 .640E+10 .640E+10 .640E+10 .982E+10 .107E+11
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IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYSED-MOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYSED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYSED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .439E+05 .171E+06 .134E+06 .263E+06 .255E+06 .132E+07 .127E+07 .333E+07 .314E+07 .302E+07 .632E+07 .671E+07
IN SOIL AIR        .381E+05 .155E+06 .132E+06 .266E+06 .269E+06 .123E+07 .126E+07 .284E+07 .292E+07 .297E+07 .508E+07 .506E+07



  LOWER SOIL ZONE:

INTO GRWATER       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
VOLATILIZED        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYSED-MOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYSED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYSED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL AIR        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00


     -- POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G) --

MOISTURE-UPPER     .172E-01 .313E-01 .336E-01 .334E-01 .325E-01 .350E-01 .344E-01 .379E-01 .368E-01 .349E-01 .397E-01 .389E-01
SOIL-UPPER         .824     1.26     1.33     1.32     1.30     1.37     1.35     1.45     1.42     1.37     1.50     1.48
AIR-UPPER          .609E-02 .125E-01 .134E-01 .134E-01 .130E-01 .140E-01 .138E-01 .152E-01 .147E-01 .140E-01 .159E-01 .156E-01
FREE LIGAND-UPPER  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00


MOISTURE-MIDDLE    .600E-05 .240E-04 .200E-04 .400E-04 .400E-04 .190E-03 .190E-03 .450E-03 .450E-03 .450E-03 .820E-03 .920E-03
SOIL-MIDDLE        .335E-02 .902E-02 .792E-02 .130E-01 .130E-01 .396E-01 .396E-01 .732E-01 .732E-01 .732E-01 .112     .122
AIR-MIDDLE         .240E-05 .961E-05 .801E-05 .160E-04 .160E-04 .761E-04 .761E-04 .180E-03 .180E-03 .180E-03 .328E-03 .368E-03
LIGAND-MIDDLE      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00


MOISTURE-LOWER     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SOIL-LOWER         .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
AIR-LOWER          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
FREE LIGAND-LOWER  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

MAX. POL.DEPTH(CM) 152.     216.     229.     271.     308.     452.     492.     651.     672.     707.     891.     933.
                            YEAR -    1 ANNUAL SUMMARY REPORT
                            ===============================


     -- TOTAL INPUTS --

UPPER SOIL ZONE                      .242E+13
MIDDLE SOIL ZONE                     .000E+00
LOWER SOIL ZONE                      .000E+00




     -- HYDROLOGIC CYCLE COMPONENTS --

AVERAGE SOIL MOISTURE( %)           10.5
TOTAL PRECIPITATION(CM)             68.5
TOTAL INFILTRATION (CM)             68.5
TOTAL EVAPOTRANSP.(CM)              52.0
TOTAL SURFACE RUNOFF(CM)            .100E-02
TOTAL GRW RUNOFF(CM)                13.0
TOTAL YIELD (CM)                    13.0
     -- POLLUTANT MASS DISTRIBUTION (UG) --

   UPPER SOIL ZONE:

TOTAL SURFACE RUNOFF                 .344E+05
TOTAL VOLATILIZED                    .221E+13
TOTAL OTHER SINKS                    .000E+00
FINAL ADS. ON SOIL                   .194E+12
FINAL IMMOBILIZED-CEC                .000E+00
TOTAL DEGRADED                       .000E+00
TOTAL HYDROLYSED-MOI                 .000E+00
TOTAL HYDROLYSED-SOI                 .000E+00
TOTAL HYDROLYSED-CEC                 .000E+00
FINAL COMPLEXED                      .000E+00
TOTAL OTHER TRANS.                   .000E+00
FINAL IN SOIL MOIST.                 .426E+09
FINAL IN SOIL AIR                    .372E+09
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   MIDDLE SOIL ZONE:

TOTAL VOLATILISED                  .000E+00
TOTAL OTHER SINKS                  .000E+00
FINAL ADS. ON SOIL                 .107E+11
FINAL IMMOBILISED-CEC              .000E+00
TOTAL DEGRADED                     .000E+00
TOTAL HYDROLYSED-MOI               .000E+00
TOTAL HYDROLYSED-SOI               .000E+00
TOTAL HYDROLYSED-CEC               .000E+00
FINAL COMPLEXED                    .000E+00
TOTAL OTHER TRANS.                 .000E+00
FINAL IN SOIL MOIST.               .671E+07
FINAL IN SOIL AIR                  .566E+07

   LOWER SOIL ZONE:

TOTAL INTO GRWATER                 .000E+00
TOTAL VOLATALISED                  .000E+00
TOTAL OTHER SINKS                  .000E+00
FINAL ADS. ON SOIL                 .000E+00
FINAL IMMOBILISED-CEC              .000E+00
TOTAL DEGRADED                     .000E+00
TOTAL HYDROLYSED-MOI               .000E+00
TOTAL HYDROLYSED-SOI               .000E+00
TOTAL HYDROLYSED-CEC               .000E+00
FINAL COMPLEXED                    .000E+00
TOTAL OTHER TRANS.                 .000E+00
FINAL IN SOIL MOIST.               .000E+00
FINAL IN SOIL AIR                  .000E+00



    -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML)OR (UG/G) --



MOISTURE-UPPER                     .338E-01
SOIL-UPPER                         1.33
AIR-UPPER                          .135E-01
FREE LIGAND-UPPER                  .000E+00


MOISTURE-MIDDLE                    .300E-03
SOIL-MIDDLE                        .403E-01
AIR-MIDDLE                         .120E-03
FREE LIGAND-MIDDLE                 .000E+00


MOISTURE-LOWER                     .000E+00
SOIL-LOWER                         .000E+00
AIR-LOWER                          .000E+00
FREE LIGAND-LOWER                  .000E+00

MAX. POL. DEPTH(M)                 9.33
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WATER BODY IS A RIVER

CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 =  1.043E+06

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  -- POLLUTANT MASS INPUT TO COLUMN(UG) --

                      OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP

PRECIPITATION      .173E+07 .139E+07 .164E+06 .898E+06 .665E+06 .257E+07 .932E+06 .239E+07 .676E+06 .607E+06 .358E+07 .113E+07
OTHER(UPPER)       .189E+12 .284E+12 .299E+12 .303E+12 .305E+12 .302E+12 .304E+12 .301E+12 .304E+12 .306E+12 .309E+12 .304E+12
OTHER(MIDDLE)      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER(LOWER)       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

TOTAL INPUT        .189E+12 .284E+12 .299E+12 .303E+12 .305E+12 .302E+12 .304E+12 .301E+12 .304E+12 .306E+12 .309E+12 .304E+12

  -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) --

 UPPER SOIL ZONE:

SURFACE RUNOFF     .803E+04 .858E+04 .834E-16 .241E+05 .594E+04 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
VOLATILIZED        .438E+11 .191E+12 .277E+12 .290E+12 .300E+12 .285E+12 .306E+12 .275E+12 .308E+12 .314E+12 .271E+12 .305E+12
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .144E+12 .235E+12 .256E+12 .259E+12 .255E+12 .268E+12 .265E+12 .283E+12 .278E+12 .268E+12 .292E+12 .288E+12
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-NOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .335E+09 .453E+09 .481E+09 .480E+09 .456E+09 .534E+09 .506E+09 .413E+09 .563E+09 .518E+09 .468E+09 .633E+09
IN SOIL AIR        .294E+09 .411E+09 .475E+09 .486E+09 .481E+09 .490E+09 .500E+09 .533E+09 .525E+09 .509E+09 .537E+09 .564E+09

 MIDDLE SOIL ZONE:

VOLATILIZED        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .281E+09 .757E+09 .665E+09 .124E+10 .124E+10 .415E+10 .415E+10 .808E+10 .808E+10 .808E+10 .131E+11 .165E+11
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-NOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .345E+05 .134E+06 .105E+06 .260E+06 .261E+06 .142E+07 .137E+07 .305E+07 .363E+07 .369E+07 .709E+07 .861E+07
IN SOIL AIR        .300E+05 .122E+06 .104E+06 .251E+06 .254E+06 .133E+07 .135E+07 .328E+07 .337E+07 .343E+07 .634E+07 .752E+07

 LOWER SOIL ZONE:

INTO GWATER        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
VOLATILIZED        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-NOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL AIR        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

  -- POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G) --

MOISTURE-UPPER     .136E-01 .270E-01 .304E-01 .308E-01 .303E-01 .335E-01 .329E-01 .350E-01 .342E-01 .327E-01 .367E-01 .362E-01
SOIL-UPPER         .697     1.14     1.34     1.35     1.33     1.30     1.38     1.37     1.35     1.30     1.41     1.40
AIR-UPPER          .545E-02 .108E-01 .122E-01 .124E-01 .121E-01 .130E-01 .128E-01 .140E-01 .137E-01 .131E-01 .147E-01 .145E-01
FREE LIGAND-UPPER  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

MOISTURE-MIDDLE    .308E-05 .128E-04 .108E-04 .260E-04 .260E-04 .130E-03 .130E-03 .330E-03 .330E-03 .330E-03 .650E-03 .759E-03
SOIL-MIDDLE        .204E-02 .550E-03 .483E-03 .902E-03 .902E-03 .302E-01 .302E-01 .587E-01 .587E-01 .587E-01 .952E-01 .105
AIR-MIDDLE         .129E-05 .401E-05 .400E-05 .861E-05 .861E-05 .521E-04 .521E-04 .132E-03 .132E-03 .132E-03 .260E-03 .308E-03
LIGAND-MIDDLE      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

MOISTURE-LOWER     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SOIL-LOWER         .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
AIR-LOWER          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
FREE LIGAND-LOWER  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

MAX. POL.DEPTH(CM) 152.     216.     230.     271.     308.     452.     483.     651.     672.     787.     891.     933.
                            YEAR -    1  ANNUAL SUMMARY REPORT
                            -------------------------------------

   -- TOTAL INPUTS --

UPPER SOIL ZONE                          .350E+13
MIDDLE SOIL ZONE                         .000E+00
LOWER SOIL ZONE                          .000E+00

   -- HYDROLOGIC CYCLE COMPONENTS --
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AVERAGE SOIL MOISTURE( %)          10.5
TOTAL PRECIPATION(CM)              68.5
TOTAL INFILTRATION (CM)            68.5
TOTAL EVAPOTRANSP.(CM)             52.0
TOTAL SURFACE RUNOFF(CM)           .188E-02
TOTAL GRW RUNOFF(CM)               13.0
TOTAL YIELD (CM)                   13.0



     -- POLLUTANT MASS DISTRIBUTION (UG) --

   UPPER SOIL ZONE:

TOTAL SURFACE RUNOFF               .474E+05
TOTAL VOLATILIZED                  .319E+13
TOTAL OTHER SINKS                  .000E+00
FINAL ADS. ON SOIL                 .298E+12
FINAL IMMOBILIZED-CEC              .000E+00
TOTAL DEGRADED                     .000E+00
TOTAL HYDROLYZED-MOI               .000E+00
TOTAL HYDROLYZED-SOI               .000E+00
TOTAL HYDROLYZED-CEC               .000E+00
FINAL COMPLEXED                    .000E+00
TOTAL OTHER TRANS.                 .000E+00
FINAL IN SOIL MOIST.               .623E+09
FINAL IN SOIL AIR                  .564E+09

   MIDDLE SOIL ZONE:

TOTAL VOLATILIZED                  .000E+00
TOTAL OTHER SINKS                  .000E+00
FINAL ADS. ON SOIL                 .145E+11
FINAL IMMOBILIZED-CEC              .000E+00
TOTAL DEGRADED                     .000E+00
TOTAL HYDROLYZED-MOI               .000E+00
TOTAL HYDROLYZED-SOI               .000E+00
TOTAL HYDROLYZED-CEC               .000E+00
FINAL COMPLEXED                    .000E+00
TOTAL OTHER TRANS.                 .000E+00
FINAL IN SOIL MOIST.               .861E+07
FINAL IN SOIL AIR                  .752E+07

   LOWER SOIL ZONE:

TOTAL INTO GRWATER                 .000E+00
TOTAL VOLATALIZED                  .000E+00
TOTAL OTHER SINKS                  .000E+00
FINAL ADS. ON SOIL                 .000E+00
FINAL IMMOBILIZED-CEC              .000E+00
TOTAL DEGRADED                     .000E+00
TOTAL HYDROLYZED-MOI               .000E+00
TOTAL HYDROLYZED-SOI               .000E+00
TOTAL HYDROLYZED-CEC               .000E+00
FINAL COMPLEXED                    .000E+00
TOTAL OTHER TRANS.                 .000E+00
FINAL IN SOIL MOIST.               .000E+00
FINAL IN SOIL AIR                  .000E+00



     -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML)OR (UG/G) --


MOISTURE-UPPER                     .316E-01
SOIL-UPPER                         1.25
AIR-UPPER                          .124E-01
FREE LIGAND-UPPER                  .000E+00


MOISTURE-MIDDLE                    .327E-03
SOIL-MIDDLE                        .390E-01
AIR-MIDDLE                         .909E-04
FREE LIGAND-MIDDLE                 .000E+00


MOISTURE-LOWER                     .000E+00
SOIL-LOWER                         .000E+00
AIR-LOWER                          .000E+00
FREE LIGAND-LOWER                  .000E+00

MAX. POL. DEPTH(M)                 9.33
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WATER BODY IS AN ESTUARY

CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 =  8.379E+07

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   -- POLLUTANT MASS INPUT TO COLUMN(UG) --


                      OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG      SEP

PRECIPITATION      .500E+08 .301E+08 .523E+07 .386E+08 .331E+08 .887E+08 .325E+08 .103E+09 .233E+09 .214E+08 .123E+09 .394E+08
OTHER(UPPER)       .935E+13 .950E+13 .971E+13 .102E+14 .106E+14 .104E+14 .106E+14 .104E+14 .106E+14 .108E+14 .104E+14 .106E+14
OTHER(MIDDLE)      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER(LOWER)       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00


TOTAL INPUT        .935E+13 .950E+13 .971E+13 .102E+14 .106E+14 .105E+14 .106E+14 .104E+14 .106E+14 .108E+14 .105E+14 .106E+14
   -- POLLUTANT MASS DISTRIBUTION IN COLUMN (UG) --

  UPPER SOIL ZONE:

SURFACE RUNOFF     .269E+06 .229E+06 .296E-16 .779E+06 .201E+06 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
VOLATILIZED        .104E+13 .405E+13 .610E+13 .965E+13 .104E+14 .970E+13 .106E+14 .993E+13 .107E+14 .110E+14 .953E+13 .106E+14
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .449E+13 .809E+13 .861E+13 .102E+14 .103E+14 .108E+14 .109E+14 .112E+14 .114E+14 .111E+14 .119E+14 .118E+14
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-MOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .560E+10 .124E+11 .149E+11 .159E+11 .157E+11 .183E+11 .176E+11 .211E+11 .197E+11 .183E+11 .230E+11 .217E+11
IN SOIL AIR        .487E+10 .112E+11 .147E+11 .161E+11 .165E+11 .171E+11 .174E+11 .180E+11 .183E+11 .180E+11 .185E+11 .190E+11

  MIDDLE SOIL ZONE:

VOLATILIZED        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .785E+10 .785E+10 .785E+10 .785E+10 .785E+10 .109E+12 .109E+12 .260E+12 .260E+12 .260E+12 .439E+12 .439E+12
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-MOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .704E+06 .684E+06 .644E+06 .633E+06 .615E+06 .268E+08 .250E+08 .998E+08 .942E+08 .905E+08 .386E+09 .197E+09
IN SOIL AIR        .613E+06 .625E+06 .636E+06 .641E+06 .648E+06 .250E+08 .254E+08 .852E+08 .874E+08 .869E+08 .167E+09 .172E+09
  LOWER SOIL ZONE:

INTO GRWATER       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
VOLATILIZED        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER SINKS        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
ADS. ON SOIL       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IMMOBILIZED-CEC    .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
DEGRADED           .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-MOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-SOI     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
HYDROLYZED-CEC     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
COMPLEXED          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
OTHER TRANS.       .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL MOIST.     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
IN SOIL AIR        .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

   -- POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G) --


MOISTURE-UPPER     .536E-02 .131E-01 .154E-01 .166E-01 .170E-01 .182E-01 .182E-01 .197E-01 .195E-01 .199E-01 .207E-01 .204E-01
SOIL-UPPER         .355     .649     .761     .898     .917     .859     .859     .900     .903     .886     .939     .938
AIR-UPPER          .213E-02 .495E-02 .614E-02 .671E-02 .681E-02 .736E-02 .736E-02 .790E-02 .763E-02 .756E-02 .837E-02 .826E-02
FREE LIGAND-UPPER  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
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MOISTURE-MIDDLE    .100E-05 .100E-05 .100E-05 .100E-05 .100E-05 .400E-04 .400E-04 .140E-03 .140E-03 .140E-03 .280E-03 .280E-03
SOIL-MIDDLE        .932E-03 .932E-03 .932E-03 .932E-03 .932E-03 .130E-01 .130E-01 .310E-01 .310E-01 .310E-01 .322E-01 .322E-01
AIR-MIDDLE         .400E-06 .400E-06 .400E-06 .460E-06 .400E-06 .160E-04 .160E-04 .561E-04 .561E-04 .561E-04 .112E-03 .112E-03
LIGAND-MIDDLE      .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

MOISTURE-LOWER     .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
SOIL-LOWER         .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
AIR-LOWER          .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00
FREE LIGAND-LOWER  .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00 .000E+00

MAX. POL.DEPTH(CM) 152.     216.     220.     271.     300.     452.     483.     651.     672.     707.     891.     933.

                           YEAR -    1  ANNUAL SUMMARY REPORT
                           ________________________________

     -- TOTAL INPUTS --

UPPER SOIL ZONE                 .119E+15
MIDDLE SOIL ZONE                .000E+00
LOWER SOIL ZONE                 .000E+00

     -- HYDROLOGIC CYCLE COMPONENTS --


AVERAGE SOIL MOISTURE( %)       10.5
TOTAL PRECIPITATION(CM)         66.5
TOTAL INFILTRATION (CM)         66.5
TOTAL EVAPOTRANSP.(CM)          53.5
TOTAL SURFACE RUNOFF(CM)        .100E-02
TOTAL GRW RUNOFF(CM)            13.0
TOTAL YIELD (CM)                13.0


     -- POLLUTANT MASS DISTRIBUTION (UG) --

   UPPER SOIL ZONE:


TOTAL SURFACE RUNOFF            .141E+07
TOTAL VOLATILIZED               .106E+15
TOTAL OTHER SINKS               .000E+00
FINAL ADS. ON SOIL              .116E+14
FINAL IMMOBILIZED-CEC           .000E+00
TOTAL DEGRADED                  .000E+00
TOTAL HYDROLYZED-MOI            .000E+00
TOTAL HYDROLYZED-SOI            .000E+00
TOTAL HYDROLYZED-CEC            .000E+00
FINAL COMPLEXED                 .000E+00
TOTAL OTHER TRANS.              .000E+00
FINAL IN SOIL MOIST.            .217E+11
FINAL IN SOIL AIR               .198E+11

   MIDDLE SOIL ZONE:


TOTAL VOLATILIZED               .000E+00
TOTAL OTHER SINKS               .000E+00
FINAL ADS. ON SOIL              .430E+12
FINAL IMMOBILIZED-CEC           .000E+00
TOTAL DEGRADED                  .000E+00
TOTAL HYDROLYZED-MOI            .000E+00
TOTAL HYDROLYZED-SOI            .000E+00
TOTAL HYDROLYZED-CEC            .000E+00
FINAL COMPLEXED                 .000E+00
TOTAL OTHER TRANS.              .000E+00
FINAL IN SOIL MOIST.            .197E+09
FINAL IN SOIL AIR               .172E+09

   LOWER SOIL ZONE:

TOTAL INTO GRWATER              .000E+00
TOTAL VOLATALIZED               .000E+00
TOTAL OTHER SINKS               .000E+00
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FINAL ADS. ON SOIL                .000E+00
FINAL IMMOBILISED-CEC             .000E+00
TOTAL DEGRADED                    .000E+00
TOTAL HYDROLYSED-MOI              .000E+00
TOTAL HYDROLYSED-SOI              .000E+00
TOTAL HYDROLYSED-CEC              .000E+00
FINAL COMPLEXED                   .000E+00
TOTAL OTHER TRANs.                .000E+00
FINAL IN SOIL MOIST.              .000E+00
FINAL IN SOIL AIR                 .000E+00




    -- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML)OR (UG/G) --



MOISTURE-UPPER                    .160E-01
SOIL-UPPER                        .895
AIR-UPPER                         .676E-02
FREE LIGAND-UPPER                 .000E+00


MOISTURE-MIDDLE                   .808E-04
SOIL-MIDDLE                       .192E-01
AIR-MIDDLE                        .355E-04
FREE LIGAND-MIDDLE                .000E+00


MOISTURE-LOWER                    .000E+00
SOIL-LOWER                        .000E+00
AIR-LOWER                         .000E+00
FREE LIGAND-LOWER                 .000E+00

MAX. POL. DEPTH(M)                9.33



****************************************EXECUTION COMPLETED****************************************
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                              MODEL FLAGS THAT DETERMINE WHAT USER INPUTS
        OPTION CHOSEN     NAME                          MEANING

               POINT     AIRFLG     SIGNIFIES AIR POINT SOURCE
                 GAS     AIRPOL     SIGNIFIES POLLUTANT IS A GAS
                 YES       LAKE     SIGNIFIES THAT A LAKE IS BEING CONSIDERED
                  NO     SEDLKE     SEDLKE = NO AND TRICON = NO SIGNIFY THAT SEDIMENT
                  NO     TRICON      PARAMETERS (FOR LAURSENS FORMULA)FOR A TRIBUTARY
                                     FLOWING INTO A LAKE ARE INPUT (SEE BELOW)
                 YES      RIVER     SIGNIFIES THAT A RIVER IS BEING CONSIDERED
                  NO     SEDRIV     SIGNIFIES THAT SEDIMENT PARAMETERS (FOR LAURSENS
                                     FORMULA) FOR THE RIVER ARE INPUT (SEE BELOW)
                 YES       ESTU     SIGNIFIES THAT AN ESTUARY IS BEING CONSIDERED
                 YES     DISFLG     SIGNIFIES THAT THE LONGITUDINAL DISPERSION
                                     COEFFICIENT (FOR ESTUARY) IS INPUT (SEE BELOW)
                 YES      OCEAN     SIGNIFIES THAT AN OCEAN IS BEING CONSIDERED
                ACID     CHMFLG     SIGNIFIES THAT CHEMICAL IS AN ACID


                                     AIR COMPARTMENT PARAMETERS INPUT

          DEFINITION                      NAME        UNIT      VALUE(S)

       WIND SPEED FOR MON=1, 6 IYR= 1   UV(MON,IYR)    M/S     5.000E+00  5.000E+00  5.000E+00  5.000E+00  5.000E+00  5.000E+00

                      MON=7,12 IYR= 1                          5.000E+00  5.000E+00  5.000E+00  5.000E+00  5.000E+00  5.000E+00

    DRY DEPOSITION VELOCITY FOR GASES      UDG         M/S     1.000E-02
            WASHOUT RATIO FOR GASES       WRATG        (-)     3.270E+00
       AIR CHEMICAL DEGRADATION RATE        AK        S**-1    1.600E-05
AIR POLLUTANT RATE FOR MON=1, 6 IYR= 1  QS(MON,IYR)    KG/S    2.200E-03  2.200E-03  2.200E-03  2.200E-03  2.200E-03  2.200E-03

                      MON=7,12 IYR= 1                          2.200E-03  2.200E-03  2.200E-03  2.200E-03  2.200E-03  2.200E-03

    MIXING HEIGHT FOR MON=1, 6 IYR= 1  HMIX(MON,IYR)    M      2.000E+03  2.000E+03  2.000E+03  2.000E+03  2.000E+03  2.000E+03

                      MON=7,12 IYR= 1                          2.000E+03  2.000E+03  2.000E+03  2.000E+03  2.000E+03  2.000E+03

                         STACK HEIGHT       HS          M      1.000E+02
       GRAVITATIONAL SETTLING VELOCITY      VS         M/S     0.000E+00
               STACK GAS EXIT VELOCITY      VE         M/S     0.000E+00
                          STACK RADIUS     SRAD         M      1.000E+01
                     STACK GAS DENSITY      RHO      KG/M**3   6.600E-01
                 ENTHALPY OF STACK GAS     ENTPY       J/KG    2.500E+05


                                     WATER COMPARTMENT PARAMETERS INPUT

          DEFINITION                      NAME        UNIT      VALUE(S)

               DISSOCIATION CONSTANT      DISK      MOLES/L   0.000E+00


LAKE :

   LAKE POLLUTANT RATE MON=1, 6 IYR= 1 WMINL(MON,IYR)  KG/S    1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

                     MON=7,12 IYR= 1                           1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

   LAKE WATER VELOCITY MON=1, 6 IYR= 1 WVELL(MON,IYR)  M/S     5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01

                     MON=7,12 IYR= 1                           5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01

                 SURFACE AREA OF LAKE    AREALK       M**2     3.750E+06
                        DEPTH OF LAKE     WDEPL        M       2.000E+00
     LENGTH OF WATERSHED OUT FROM LAKE    XSOIL        M       5.000E+02

      PHOTOLYSIS RATE CONSTANT (WATER)     WKPL      S**-1     6.200E-08
      HYDROLYSIS RATE CONSTANT (WATER)     WKHL      S**-1     0.000E+00
       OXIDATION RATE CONSTANT (WATER)     WKOL      S**-1     0.000E+00
  BIODEGRADATION RATE CONSTANT (WATER)     WKBL      S**-1     0.000E+00
  VOLATILIZATION RATE CONSTANT (WATER)     WKVL      S**-1     5.560E-05
     SOIL-WATER PARTITION COEFFICIENT    SWLSWL  MOL/KG/MOL/L  1.500E+01
MEDIAN SEDIMENT DIAMETER IN TRIBUTARY    DIASDT       MM       4.500E-01
      SEDIMENT DENSITY IN TRIBUTARY      DENSDT    G/CM**3     2.650E+00
         WATER DENSITY IN TRIBUTARY       DENWT    G/CM**3     1.000E+00
                 DEPTH OF TRIBUTARY       WDEPT       M        2.000E+00
                 SLOPE OF TRIBUTARY      SLOPET      (-)       1.000E-04
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RIVER :

  RIVER POLLUTANT RATE MON=1, 6 ITR= 1 WKINR(MON,ITR)  KG/S     1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

                      MON=7,12 ITR= 1                           1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

  RIVER WATER VELOCITY MON=1, 6 ITR= 1 WVELR(MON,ITR)  M/S      1.500E+00  1.500E+00  1.500E+00  1.500E+00  1.500E+00  1.500E+00

                      MON=7,12 ITR= 1                           1.500E+00  1.500E+00  1.500E+00  1.500E+00  1.500E+00  1.500E+00

                     NUMBER OF REACHES      NR          (-)             3
                  LENGTH OF RIVER REACH     WLENR        M      5.000E+02
                   WIDTH OF RIVER REACH     WWIDR        M      3.000E+02
                   DEPTH OF RIVER REACH     WDEPR        M      1.000E+01

       PHOTOLYSIS RATE CONSTANT (WATER)     WKPR       S**-1    6.200E-08
       HYDROLYSIS RATE CONSTANT (WATER)     WKHR       S**-1    0.000E+00
        OXIDATION RATE CONSTANT (WATER)     WKOR       S**-1    0.000E+00
   BIODEGRADATION RATE CONSTANT (WATER)     WKBR       S**-1    0.000E+00
   VOLATILISATION RATE CONSTANT (WATER)     WKVR       S**-1    5.560E-05
       SOIL-WATER PARTITION COEFFICIENT     SWKSWR   MOL/KG/MOL/L 1.500E+01
     MEDIAN SEDIMENT DIAMETER IN RIVER      DIASDR       MM     4.500E-01
          SEDIMENT DENSITY IN RIVER         DENSDR    G/CM**3   2.650E+00
             WATER DENSITY IN RIVER         DLWR      G/CM**3   1.000E+00
                     SLOPE OF RIVER         SLOPER      (-)     7.500E-05


ESTUARY :

ESTUARY POLLUTANT RATE MON=1, 6 ITR= 1  WKINE(MON,ITR)  KG/S   1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

                     MON=7,12 ITR= 1                           1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

   FRESH WATER VELOCITY MON=1, 6 ITR= 1  WVELE(MON,ITR)  M/S   5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01

                     MON=7,12 ITR= 1                           5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01

 #PTS UP & DOWNSTREAM OF SOURCE(OUTPUT)     NPTSE       (-)            2
                      LENGTH OF ESTUARY     WLENE        M     2.500E+04
                       WIDTH OF ESTUARY     WWIDE        M     1.500E+02
                       DEPTH OF ESTUARY     WDEPE        M     2.000E+00
     LONGITUDINAL DISPERSION COEFFICIENT     EL        M**2/S  7.500E+01

       PHOTOLYSIS RATE CONSTANT (WATER)     WKPE       S**-1   6.200E-08
       HYDROLYSIS RATE CONSTANT (WATER)     WKHE       S**-1   0.000E+00
        OXIDATION RATE CONSTANT (WATER)     WKOE       S**-1   0.000E+00
   BIODEGRADATION RATE CONSTANT (WATER)     WKBE       S**-1   0.000E+00
   VOLATILISATION RATE CONSTANT (WATER)     WKVE       S**-1   5.560E-05
       SOIL-WATER PARTITION COEFFICIENT    SWKSWE  MOL/KG/MOL/L 1.500E+01
SEDIMENT CONC.(ESTUARY) MON=1,6 ITR= 1  SEDCE(MON,ITR) KG/M**3 2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02

                     MON=7,12 ITR= 1                           2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02

OCEAN :

0.02*CONC. OF EFFLUENT MON=1, 6 ITR= 1  WCINO(MON,ITR) KG/M**3 1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

                     MON=7,12 ITR= 1                           1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02  1.000E-02

OCEAN CURRENT VELOCITY MON=1, 6 ITR= 1  WVELO(MON,ITR)  M/S    5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01

                     MON=7,12 ITR= 1                           5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01  5.000E-01

                 LENGTH OF LINE SOURCE      BO           M     5.000E+00
DISTANCE BETWEEN POINTS IN OCEAN OUTPUT    XOCEAN        M     5.000E+02

       PHOTOLYSIS RATE CONSTANT (WATER)     WKPO       S**-1   6.200E-08
       HYDROLYSIS RATE CONSTANT (WATER)     WKHO       S**-1   0.000E+00
        OXIDATION RATE CONSTANT (WATER)     WKOO       S**-1   0.000E+00
   BIODEGRADATION RATE CONSTANT (WATER)     WKBO       S**-1   0.000E+00
   VOLATILISATION RATE CONSTANT (WATER)     WKVO       S**-1   5.560E-05
       SOIL-WATER PARTITION COEFFICIENT    SWKSWO  MOL/KG/MOL/L 1.500E+01
 NUMBER OF POINTS FROM SOURCE (OUTPUT)     NPTSO        (-)            3
SEDIMENT CONC. (OCEAN) MON=1, 6 ITR= 1 SEDCO(MON,ITR) KG/M**3 2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02

                     MON=7,12 ITR= 1                          2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02  2.500E-02
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                                              SCENARIO

                                        TYPE OF SOURCE TERMS
                                           AIR       - POINT

                                           WATER BODY(IES) CONSIDERED:
                                                     - LAKE (HAS SOURCE)
                                                     - RIVER (HAS SOURCE)
                                                     - ESTUARY (HAS SOURCE)
                                                     - OCEAN (HAS SOURCE)
                                           UPPER SOIL - NONE
                                           MIDDLE SOIL - NONE
                                           LOWER SOIL - NONE


                                        GEOGRAPHIC REGION - CLINTON,MASS.(40 YR AVERAGED DATA FOR TEST ONLY)

                                        MAGNITUDE OF SOURCE(S)

              OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG       SEP

  AIR
(KG/SEC)
 YEAR  1   2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03  2.20E-03

LAKE
(KG/SEC)
 YEAR  1   1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02

RIVER
(KG/SEC)
 YEAR  1   1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02

ESTUARY
(KG/SEC)
 YEAR  1   1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02

OCEAN
(KG/M**2)
 YEAR  1   1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02  1.00E-02
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                              MONTHLY POLLUTANT CONCENTRATIONS AND INTERACTION TERMS

                                              WATER BODY IS A LAKE

                              CONTAMINATED WATER (SURFACE AREA) IN M**2  =  3.750E+04
                              CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 =  8.625E+05

                                                    YEAR  1
     OCT
    CONCS    MAXIMUM AIR    AVERAGE AIR     WAT NEUTRAL  WAT IONIC    WAT ADSORBED  UPPER SOIL   MIDDLE SOIL  LOWER SOIL   RESUSPENSION
  (UG/M**3)   1.396E+01      1.131E+01       4.426E+03   0.000E+00     2.293E-02    1.091E+06    4.427E+03    0.000E+00    0.000E+00
    RATES    DEP ON WATER   DEP ON SOIL     VOLAT WATER  VOLAT SOIL   SURF RUNOFF   GENTR RUNOFF WASHLOAD
  (UG/MON)    9.959E+11      1.651E+11       4.769E+12   3.096E+10     7.264E+03    0.000E+00    8.272E+06
                                                           .
                                                           .
                                                           .
     SEP
    CONCS    MAXIMUM AIR    AVERAGE AIR     WAT NEUTRAL  WAT IONIC    WAT ADSORBED  UPPER SOIL   MIDDLE SOIL  LOWER SOIL   RESUSPENSION
  (UG/M**3)   1.424E+01      1.158E+01       4.433E+03   0.000E+00     2.395E-02    1.956E+06    1.613E+05    0.000E+00    0.000E+00
    RATES    DEP ON WATER   DEP ON SOIL     VOLAT WATER  VOLAT SOIL   SURF RUNOFF   GENTR RUNOFF WASHLOAD
  (UG/MON)    1.125E+12      2.071E+11       4.791E+12   2.009E+11     0.000E+00    0.000E+00    3.300E+07
```

FOR15.DAT

```
                              MONTHLY POLLUTANT CONCENTRATIONS AND INTERACTION TERMS

                                                WATER BODY IS A RIVER
                                                IR IS THE REACH NUMBER

                              CONTAMINATED WATER (SURFACE AREA) IN M**2  =  4.500E+05
                              CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 =  1.043E+06

                                                       YEAR  1
    OCT
   CONCS    MAXIMUM AIR    AVERAGE AIR       WAT NEUTRAL   WAT IONIC   WAT ADSORBED  UPPER SOIL   MIDDLE SOIL  LOWER SOIL  RESUSPENSION
 (UG/M**3)   1.182E+01       1.012E+01 IR= 1 2.185E+03    0.000E+00    2.875E-01    9.224E+05    2.650E+03   0.000E+00    0.000E+00
                                       IR= 2 2.148E+03    0.000E+00    2.826E-01
                                       IR= 3 2.112E+03    0.000E+00    2.779E-01
   RATES    DEP ON WATER   DEP ON SOIL        VOLAT WATER  VOLAT SOIL  SURF RUNOFF   GRNTR RUNOFF  WASHLOAD
 (UG/MON)    1.018E+11      2.161E+11          1.255E+12   4.383E+10    8.830E+03    9.899E+00    1.088E+07
                                                                .
                                                                .
                                                                .
    SEP
   CONCS    MAXIMUM AIR    AVERAGE AIR       WAT NEUTRAL   WAT IONIC   WAT ADSORBED  UPPER SOIL   MIDDLE SOIL  LOWER SOIL  RESUSPENSION
 (UG/M**3)   1.293E+01       1.125E+01 IR= 1 2.185E+03    0.000E+00    2.875E-01    1.038E+06    1.394E+05   0.000E+00    0.000E+00
                                       IR= 2 2.148E+03    0.000E+00    2.829E-01
                                       IR= 3 2.114E+03    0.000E+00    2.781E-01
   RATES    DEP ON WATER   DEP ON SOIL        VOLAT WATER  VOLAT SOIL  SURF RUNOFF   GRNTR RUNOFF  WASHLOAD
 (UG/MON)    1.311E+11      3.048E+11          1.394E+12   3.851E+11    0.000E+00    0.000E+00    4.094E+07
```

FOR16.DAT

```
                          MONTHLY POLLUTANT CONCENTRATIONS AND INTERACTION TERMS

                                         WATER BODY IS AN ESTUARY
                   X IS DISTANCE FROM SOURCE IN METERS; + FOR DOWNSTREAM AND - FOR UPSTREAM

                            CONTAMINATED WATER (SURFACE AREA) IN M**2  =  3.750E+06
                            CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 =  6.379E+07

                                                  YEAR  1
    OCT
   CONCS     MAXIMUM AIR    AVERAGE AIR       WAT NEUTRAL  WAT IONIC   WAT ADSORBED  UPPER SOIL  MIDDLE SOIL  LOWER SOIL  RESUSPENSIO
 (UG/M**3)    7.944E+00      4.62E+00 X=      0 6.495E+04 0.000E+00     2.436E+01    4.702E+05    1.231E+03   0.000E+00   0.000E+00
                                      X=   6250 3.290E+04 0.000E+00     1.237E+01
                                      X=  -6250 4.264E+02 0.000E+00     1.599E-01
                                      X=  12500 1.685E+04 0.000E+00     6.317E+00
                                      X= -12500 4.264E+02 0.000E+00     1.599E-01
   RATES     DEP ON WATER   DEP ON SOIL        VOLAT WATER VOLAT SOIL   SURF RUNOFF  GRNWTR RUNOFF  WASHLOAD
 (UG/MON)     8.323E+11      6.347E+12          2.019E+13   1.036E+12   3.007E+05    0.000E+00    3.352E+08
                                                                 .
                                                                 .
                                                                 .
    SEP
   CONCS     MAXIMUM AIR    AVERAGE AIR       WAT NEUTRAL  WAT IONIC   WAT ADSORBED  UPPER SOIL  MIDDLE SOIL  LOWER SOIL  RESUSPENSIO
 (UG/M**3)    9.571E+00      6.45E+00 X=      0 6.510E+04 0.000E+00     2.441E+01    1.242E+06    6.894E+04   0.000E+00   0.000E+00
                                      X=   6250 3.313E+04 0.000E+00     1.242E+01
                                      X=  -6250 5.011E+02 0.000E+00     2.179E-01
                                      X=  12500 1.706E+04 0.000E+00     6.375E+00
                                      X= -12500 5.011E+02 0.000E+00     2.179E-01
   RATES     DEP ON WATER   DEP ON SOIL        VOLAT WATER VOLAT SOIL   SURF RUNOFF  GRNWTR RUNOFF  WASHLOAD
 (UG/MON)     6.249E+11      1.962E+13          2.003E+13   1.057E+13   0.000E+00    0.000E+00    1.995E+08
```

FOR17.DAT

```
                      MONTHLY POLLUTANT CONCENTRATIONS

                          WATER BODY IS AN OCEAN
                    X IS DISTANCE FROM SOURCE IN METERS

                                  YEAR  1
                         CONCENTRATIONS (UG/M**3)

              WATER (NEUTRAL)   WATER (IONIC)   WATER (ADSORBED)
OCT
    X=  0.50E+03   3.816E+06        0.000E+00         1.431E+03
    X=  0.10E+04   1.856E+06        0.000E+00         6.959E+02
    X=  0.15E+04   1.108E+06        0.000E+00         4.156E+02
                              .
                              .
                              .
SEP
    X=  0.50E+03   3.816E+06        0.000E+00         1.431E+03
    X=  0.10E+04   1.856E+06        0.000E+00         6.959E+02
    X=  0.15E+04   1.108E+06        0.000E+00         4.156E+02
```

FOR19.DAT

```
                          FOOD CHAIN BIOACCUMULATION FLAG

         OPTION CHOSEN *     NAME                  MEANING

                   NO        COVFLG     SIGNIFIES COMPOUND IS NOT A COVALENTLY BONDING MATERIAL



                          FOOD CHAIN BIOACCUMULATION PARAMETERS

                DEFINITION                        NAME       UNIT        VALUE

      N-OCTANOL WATER PARTITION COEFFICIENT        KOW        (-)       1.000E+02
           INITIAL INTERCEPTION FRACTION            R         (-)       4.000E-01
                   FORAGE PRODUCTIVITY             YV       G/M**2     1.500E+02
                   WEATHERING CONSTANT           LAMBDA    DAY**-1     2.500E-02
     GROWTH PERIOD OF FORAGE BEFORE HARVEST        TE         DAY       3.000E+01
          SOIL WATER PARTITION COEFFICIENT         KD         (-)       1.500E+01


                             BIOACCUMULATION FACTORS:

     BCFAQ (AQUATIC) = CONC. IN TISSUE (FRESH WT.)/CONC. IN WATER  (ML/G) =  4.000E+00
     BCFPL (PLANT) = CONC. IN TISSUE (DRY WT.)/CONC. IN SOIL  (UNITLESS) =  1.443E+00

     BCFAN (ANIMAL) = CONC. IN TISSUE (FRESH WT.)/CONC. IN DIET  (UNITLESS):
                    * BCFAN OF THE COMPOUND IS LIKELY TO BE LESS THAN 0.1



              * CONCENTRATIONS IN AQUATIC ORGANISMS AND TERRESTRIAL PLANTS (FORAGE) IN UG/G

              LAKE                          RIVER                        ESTUARY               OCEAN      SOIL-AIR OPTION
        AQUATIC      PLANTS           AQUATIC      PLANTS          AQUATIC      PLANTS        AQUATIC         PLANTS

 OCT   2.125E-02   2.639E+02        1.049E-02   2.194E+02       3.119E-01   1.054E+02      1.833E+01      0.000E+00
 NOV   2.127E-02   3.272E+02        1.049E-02   2.903E+02       3.122E-01   1.449E+02      1.833E+01      0.000E+00
 DEC   2.128E-02   3.300E+02        1.049E-02   3.044E+02       3.124E-01   1.630E+02      1.833E+01      0.000E+00
 JAN   2.128E-02   3.315E+02        1.049E-02   3.083E+02       3.126E-01   1.710E+02      1.833E+01      0.000E+00
 FEB   2.128E-02   3.317E+02        1.049E-02   3.096E+02       3.126E-01   1.763E+02      1.833E+01      0.000E+00
 MAR   2.128E-02   3.309E+02        1.049E-02   3.066E+02       3.126E-01   1.735E+02      1.833E+01      0.000E+00
 APR   2.128E-02   3.316E+02        1.049E-02   3.093E+02       3.126E-01   1.771E+02      1.833E+01      0.000E+00
 MAY   2.127E-02   3.300E+02        1.049E-02   3.059E+02       3.125E-01   1.728E+02      1.833E+01      0.000E+00
 JUN   2.128E-02   3.316E+02        1.049E-02   3.097E+02       3.126E-01   1.776E+02      1.833E+01      0.000E+00
 JUL   2.128E-02   3.320E+02        1.049E-02   3.107E+02       3.126E-01   1.790E+02      1.833E+01      0.000E+00
 AUG   2.127E-02   3.306E+02        1.049E-02   3.050E+02       3.125E-01   1.721E+02      1.833E+01      0.000E+00
 SEP   2.128E-02   3.318E+02        1.049E-02   3.092E+02       3.126E-01   1.770E+02      1.833E+01      0.000E+00
```

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* CAUTION

NO CONFIDENCE SHOULD BE PLACED IN THE METHODS USED TO CALCULATE CONCENTRATION IN AQUATIC ORGANISMS OR IN TERRESTRIAL PLANTS VIA ROOT UPTAKE, OR TO EVALUATE BIOACCUMULATION POTENTIAL IN TERRESTRIAL ANIMALS, IF:

1) THE COMPOUND IS A COVALENTLY BONDING COMPOUND,
2) THE COMPOUND IS APPRECIABLY DEGRADED IN THE BIOTIC PHASE,
3) THE DOMINANT CONCENTRATING PHASE IN THE ORGANISM IS NOT A LIPID,
4) THE KOW EQUALS OR EXCEEDS 1.0E+6, OR IF
5) THE CALCULATED BCF VALUE IS BELOW 10.

IT SHOULD FURTHER BE RECOGNIZED THAT THE METHOD IS NOT ABSOLUTE BECAUSE STERIC PROPERTIES AND SIZE OF THE CHEMICAL COMPOUND, IN ADDITION TO LIPOPHILICITY, AFFECT THE PREDICTED ACCUMULATION IN TISSUES. ALSO, A POSSIBLY SIGNIFICANT DEGREE OF UNCERTAINTY SHOULD BE ATTACHED TO ESTIMATED CONCENTRATIONS FOR ANY ONE ORGANISM DUE TO DIFFERENCES IN FRACTIONAL LIPID COMPOSITION.

APPENDIX E

LISTING OF TOX-SCREEN (INCLUDES SESOIL PORTION WHICH HAS BEEN ADAPTED)

The MAIN program is listed first followed by the TOX-SCREEN routines in alphabetical order. These routines are then followed by the SESOIL routines (in alphabetical order) which have been adapted for TOX-SCREEN. Finally, a listing of the general purpose integrator package D01AJF is included at the end of this appendix.

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```
C
C                             TOX-SCREEN
C                  MULTIMEDIA SCREENING-LEVEL MODEL
C               D.M. HETRICK AND L.M. MCDOWELL-BOYER
C                    OAK RIDGE NATIONAL LABORATORY
C                             JULY, 1982
C   DEVELOPED TO ASSESS THE POTENTIAL FOR ENVIRONMENTAL ACCUMULATION OF
C   CHEMICALS RELEASED TO AIR, SURFACE WATER, OR SOIL. SOIL MODEL SESOIL
C   (BONAZOUNTAS AND WAGNER, 1981 FROM A.D. LITTLE) WAS ADAPTED FOR THIS
C   MODEL. THIS PROGRAM WAS DEVELOPED AT THE REQUEST OF THE U.S.
C   ENVIRONMENTAL PROTECTION AGENCY.
C
C   SESOIL-82 (MAIN PROGRAM)
C
      REAL NUT1,LOAD
      COMMON /TI/ TITLES(5,12)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /HYM/ CLIMM1(6,12,10),CLIMM2(6,12,10),CLIMM3(12,10)
      COMMON /NU/ NUT1(6)
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12)
      COMMON /HB/ HYDBAL(13,10)
      COMMON /FI/ IOR,IOW,IGE,IL0,IL1,IL2,IL3
      REAL LIGU,LIGM,LIGL,IA
      COMMON /LEV2/PCONC(13,15,3),THM,LIGU,LIGL,LIGM
      COMMON /HYR/ THA,PA,IA,ETA,RSA,RGA,YA,GZ,SIGMA,FGAM,G,XI
      COMMON/CAVPAR/HEFFIV,XMAX,HMIXS,U,VG,UDPW,DEPFAC
      COMMON/MEDIA/AWMINR,AWMOUR,WAMOUR(20),AWMINL,AWMOUL,
     $             WAMOUL,SWMINL,SWMINR,AWMINE,AWMOUE,SWMINE,WAMOUE,
     $             SAMOUL,ASMIDL,ASMIWL,SAMOUR,ASMIDR,ASMIWR,SAMOUE,
     $             ASMIDE,ASMIWE,ASMOWL,ASMODL,ASMODR,ASMOWR,
     $             ASMODE,ASMOWE,SWMOUL,SWMOUR,SWMOUE,CUMLKE,
     $             CLMLKE,CUMRIV,CLMRIV,CUMEST,CLMEST,ASMODS,ASMOWS,
     $             ASMIDS,ASMIWS,SAMOUS,CUMS,CLMS,SUMLKE,SLMLKE,CUSALK,
     $             CLSALK,LIGCUL,LIGCLL,SUMRIV,SLMRIV,CUSARV,CLSARV,
     $             LIGCUR,LIGCLR,SUMEST,SLMEST,CUSAES,CLSAES,LIGCUE,
     $             LIGCLE,SUMS,SLMS,CUSAS,CLSAS,LIGCUS,LIGCLS,CMMLKE,
     $             CMMRIV,CMMEST,CMMS,SMMLKE,SMMRIV,SMMEST,SMMS,
     $             CMSALK,CMSARV,CMSAES,CMSAS,LIGCML,LIGCMR,LIGCME,
     $             LIGCMS
      COMMON/WPARL/WVELL(12,10),WMINL(12,10),WMTLKE,AREALK,
     $             WDEPL,WVOLL
      COMMON/WPARR/WVELR(12,10),WMINR(12,10),WMTRIV(20),
     $             NR,WWIDR,WLENR,WDEPR,WVOLR,WMTOLD,AREAR
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $             ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      DATA YES/4H YES/
C
C --- FILE NUMBERS
C
      IGE=1
      IL3=2
      IOR=5
      IOW=6
```

```
C
C --- RUN FOR EACH EXECUTION CARD
C
   10 CONTINUE
C
C ----- INITIALIZE ARRAYS-----
C
C
      DO 8 I=1,6
      DO 8 J=1,12
      DO 8 K=1,10
      CLIMM1(I,J,K)=0.0
    8 CLIMM2(I,J,K)=0.0
      DO 9 I=1,12
      DO 9 J=1,10
    9 CLIMM3(I,J)=0.0
C
      DO 4 I=1,6
      SOIL1(I)=0.0
      SOIL2(I)=0.0
      NUT1(I)=0.0
      LOAD(I)=0.0
      RUNLO(I)=0.0
    4 CONTINUE
C
      DO 6 I=1,18
      CHEM1(I)=0.0
    6 CONTINUE
C
      DO 7 I=1,20
      GEOM(I)=0.0
    7 CONTINUE
C
      DO 5 J=1,10
      DO 5 I=1,12
      RUNM1(J,I)=0.0
      RUNM2(J,I)=0.0
    5 CONTINUE
C
C --- READ EXECUTION CARD
C
      READ(IOR,904)JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
  904 FORMAT(8I5)
C
C --- IF LAST CARD, GO TO END
C
      IF(JRUN .GE. 999)GO TO 999
C
C --- OTHERWISE EXECUTE RUN
C
C --- READ DATA FOR ONE RUN AT A TIME
C
      CALL RFILE
      CALL READIN
      IF(RIVER.NE.YES)GO TO 20
```

```
C
C --- INITIALIZE VARIABLES FOR EACH WATER BODY TYPE (VOLATILIZATION TERMS,
C --- DEPOSITION TERMS, ETC.)
C
      DO 30 I=1,NR
      WAMOUR(I)=0.0
 30   WMTRIV(I)=0.0
 20   WMTLKE=0.0
      WMTOLD=0.0
      WAMOUL=0.0
      AWMOUL=0.0
      AWMOUR=0.0
      WAMOUE=0.0
      AWMOUE=0.0
      ASMOWL=0.0
      ASMODL=0.0
      SAMOUL=0.0
      SAMOUR=0.0
      ASMODR=0.0
      ASMOWR=0.0
      SAMOUE=0.0
      ASMODE=0.0
      ASMOWE=0.0
      SWMOUL=0.0
      SWMOUR=0.0
      SWMOUE=0.0
      CUMLKE=0.0
      CLMLKE=0.0
      CUMRIV=0.0
      CLMRIV=0.0
      CUMEST=0.0
      CLMEST=0.0
      CUMS=0.0
      CLMS=0.0
      ASMODS=0.0
      ASMOWS=0.0
      SAMOUS=0.0
      SUMLKE=0.0
      SLMLKE=0.0
      CUSALK=0.0
      CLSALK=0.0
      LIGCUL=0.0
      LIGCLL=0.0
      SUMRIV=0.0
      SLMRIV=0.0
      CUSARV=0.0
      CLSARV=0.0
      LIGCUR=0.0
      LIGCLR=0.0
      SUMEST=0.0
      SLMEST=0.0
      CUSAES=0.0
      CLSAES=0.0
      LIGCUE=0.0
      LIGCLE=0.0
      SUMS=0.0
      SLMS=0.0
      CUSAS=0.0
      CLSAS=0.0
      LIGCUS=0.0
      LIGCLS=0.0
      CMMLKE=0.0
      CMMRIV=0.0
      CMMEST=0.0
      CMMS=0.0
      SMMLKE=0.0
      SMMRIV=0.0
      SMMEST=0.0
      SMMS=0.0
      CMSALK=0.0
      CMSARV=0.0
      CMSAES=0.0
      CMSAS=0.0
      LIGCML=0.0
      LIGCMR=0.0
      LIGCME=0.0
      LIGCMS=0.0
C
C --- CALL ROUTINES  FOR EXECUTION LEVEL
C
      IF(LEVEL .EQ.3)CALL LEVEL3
C
C --- END OF EXECUTION -STOP
C
  999 STOP
      END
      SUBROUTINE AIR(IMON,IYR,ISTEP,NSTEPS,DT)
      COMMON/MEDIA/AWMINR,AWMOUR,WAMOUR(20),AWMINL,AWMOUL,
     $           WAMOUL,SWMINL,SWMINR,AWMINE,AWMOUE,SWMINE,WAMOUE,
     $           SAMOUL,ASMIDL,ASMIWL,SAMOUR,ASMIDR,ASMIWR,SAMOUE,
     $           ASMIDE,ASMIWE,ASMOWL,ASMODL,ASMODR,ASMOWR,
     $           ASMODE,ASMOWE,SWMOUL,SWMOUR,SWMOUE,CUMLKE,
     $           CLMLKE,CUMRIV,CLMRIV,CUMEST,CLMEST,ASMODS,ASMOWS,
     $           ASMIDS,ASMIWS,SAMOUS,CUMS,CLMS,SUMLKE,SLMLKE,CUSALK,
     $           CLSALK,LIGCUL,LIGCLL,SUMRIV,SLMRIV,CUSARV,CLSARV,
     $           LIGCUR,LIGCLR,SUMEST,SLMEST,CUSAES,CLSAES,LIGCUE,
     $           LIGCLE,SUMS,SLMS,CUSAS,CLSAS,LIGCUS,LIGCLS,CMMLKE,
     $           CMMRIV,CMMEST,CMMS,SMMLKE,SMMRIV,SMMEST,SMMS,
     $           CMSALK,CMSARV,CMSAES,CMSAS,LIGCML,LIGCMR,LIGCME,
     $           LIGCMS
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $           ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/ALPHAS/A1L,A2L,A3L,A1R,A2R,A3R,A1E,A2E,A3E,
     $            A1O,A2O,A3O
      COMMON/AIRPAR/QS(12,10),UW(12,10),HMIX(12,10),CTYLTH,
     $            UDG,UDP,WRATG,WRATP,AK,HS,VS,SRAD,RHO,ENTPY
      COMMON/WPARL/WVELL(12,10),WMINL(12,10),WMTLKE,AREALK,
     $           WDEPL,WVOLL
      COMMON/WPARR/WVELR(12,10),WMINR(12,10),WMTRIV(20),
     $           NR,WWIDR,WLENR,WDEPR,WVOLR,WMTOLD,AREAR
      COMMON/WPARE/WVELE(12,10),WMINE(12,10),TIDMAX,EL,WWIDE,
     $           WLENE,WDEPE,NPTSE,AREAE
      COMMON/CAVPAR/HEFFIV,XMAX,HMIXE,U,VG,UDPW,DEPFAC
      COMMON/SPARS/ARS,AREAS,XLENS
      COMMON/SPARL/ARL,AREASL,XSOIL
      COMMON/SPARR/ARR,AREASR
      COMMON/SPARE/ARE,AREASE
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12)
      COMMON /HB/ HYDBAL(13,10)
      COMMON/OUT/ACMAXL,AVAIRL,AVAIRR,AVAIRE,AWDEPL,AWDEPR,AWDEPE,
     $         ASDEPL,ASDEPR,ASDEPE,WVOLAL,WVOLAR,WVOLAE,SVOLAL,
     $         SVOLAR,SVOLAE,SWSURL,SWSURR,SWSURE,SWGRWL,SWGRWR,
     $         SWGRWE,SCONUL,SCONUR,SCONUE,SCONLL,SCONLR,SCONLE,
     $         CONL1,CONL2,CONL3,CONR1(20),CONR2(20),CONR3(20),
     $         CNCED1(11),CNCED2(11),CNCED3(11),CNCEU1(11),CNCEU2(11),
     $         CNCEU3(11),XESTY(11),CONO1(10),CONO2(10),CONO3(10),
     $         RESUSE,WASHL,WASHR,WASHE,ACMAXR,ACMAXE,ACMAXS,
     $         AVAIRS,ASDEPS,SVOLAS,SWGRWS,SCONUS,SCONLS,RESUSS,
     $         RESUSL,RESUSR,SCONML,SCONMR,SCONME,SCONMS,SWSURS,
     $         WASHS,AREA1(3)
      REAL NONE,LAKE,NO
      DIMENSION HEFF(18),XMXEFF(18),WORK(800),IWORK(102)
      EXTERNAL CAVGE
      EXTERNAL DEPAVG
      DATA HEFF/7.,8.,10.,15.,20.,30.,40.,50.,60.,70.,
     $          100.,150.,200.,250.,300.,350.,400.,450./
C
C DATA IN XMXEFF ARE LN (#'S) IN GRAPH IN DOCUMENT (HEFF AND XMXEFF
C ARE USED IN COMPUTING XMAX AND HEFFIV BELOW)
C
      DATA XMXEFF/-2.254,-2.096,-1.833,-1.374,-1.050,-.58,
     $          -.248,.02,.30,.604,1.065,1.723,2.197,2.565,2.862,
     $            3.157,3.434,3.75/
      DATA EPS/1.0/
      DATA AREA/4HAREA/,GAS/4H GAS/,YES/4H YES/,POINT/4HPOIN/
      DATA NONE/4HNONE/,PI/3.1415927/,NO/4H  NO/
C
      IWP=13
      MON=IMON
      IF(ISTEP.GT.1)GO TO 225
      IF(AIRFLG.EQ.NONE)GO TO 140
      IF(AIRFLG.EQ.AREA)GO TO 5
      IF(AIRFLG.EQ.POINT)GO TO 10
C
C  AREA SOURCE
C QS IS MONTHLY SOURCE STRENGTH (KG/S), CTYLTH IS LENGTH OF
C URBAN AREA (M), UW IS WIND SPEED (M/S), AK IS AIR CHEMICAL
C RATE CONSTANT (S**-1)
C
 5    DEDGE=0.5*CTYLTH
      C=SQRT(2.0/PI)*DEDGE**.25/0.0375
      ACMAX=C*QS(MON,IYR)/(CTYLTH*CTYLTH*UW(MON,IYR))
      IF(AK.EQ.0.0)GO TO 150
      ACMAX=ACMAX*EXP(-DEDGE*AK/UW(MON,IYR))
      GO TO 150
C
C  POINT SOURCE
C  F IS HEAT FLUX (M**4/S**3), UW WIND SPEED (M/S), HS STACK HEIGHT (M)
C  QS IS MONTHLY SOURCE STRENGTH (KG/S)
C
 10   CONTINUE
C
C QH IS IN WATTS (JOULES/SEC), 4.184 CONVERTS TO CAL/SEC NEEDED IN
C F BELOW. THE FOLLOWING IS USED TO COMPUTE XMAX AND HEFFIV (DEFINED BELOW)
C
      IF(RHO.EQ.0.0.OR.ENTPY.EQ.0.0)GO TO 20
      QH=VS*PI*SRAD*SRAD*RHO*ENTPY/4.184
      F=3.7E-5*QH
      GO TO 23
 20   F=G*VS*SRAD*SRAD
 23   CONTINUE
      FP=F**0.4
      IF(HS.GT.300.0)XSTAR=67.31*FP
      IF(HS.LE.300.0)XSTAR=2.164*FP*(HS**0.6)
      FDUW=1.60*(F**0.3333333)/UW(MON,IYR)
      XMAX=5.6
      HOLD=150.0
 25   XMAX=XMAX*1000.0
      DH=FDUW*XMAX**0.6666667
      IF(XSTAR.EQ.0.0)GO TO 30
      XMXDXS=XMAX/XSTAR
      IF(XMXDXS.GT.1.0)DH=FDUW*(XSTAR**0.6666667)*(0.4+0.64*XMXDXS+
     $    2.2*XMXDXS*XMXDXS)/(1.0+0.8*XMXDXS)**2
C
C  HSPDH IS EFFECTIVE STACK HEIGHT; ASSUME 7.LE.HSPDH.LE.450 METERS
C
 30   HSPDH=HS+DH
      IF(ABS(HSPDH-HOLD).LT.EPS)GO TO 100
      HOLD=HSPDH
      IF(HOLD.LT.HEFF(1))GO TO 60
      DO 50 I=1,17
   50 IF(HOLD.GE.HEFF(I).AND.HOLD.LT.HEFF(I+1))GO TO 75
      XMAX=EXP(XMXEFF(18))
      J=18
      GO TO 25
   60 J=1
      XMAX=EXP(XMXEFF(1))
      GO TO 25
   75 DELTA=(HOLD-HEFF(I))/(HEFF(I+1)-HEFF(I))
      XMAX=EXP(XMXEFF(I)+(XMXEFF(I+1)-XMXEFF(I))*DELTA)
      J=I
      GO TO 25
  100 IF((J.EQ.18).OR.(J.EQ.1.AND.HOLD.LT.HEFF(1)))GO TO 110
      GO TO 130
  110 CONTINUE
      WRITE(IWP,125)
  125 FORMAT(1X,'WARNING IN AIR : HEFF OUTSIDE THE BOUNDS OF AVAILABLE D
     $ATA; CODE USED DATA AT ENDPOINT FOR XMAX ')
  130 HEFFIV=HOLD
C
C XMAX IS X MAXIMUM (M) - DISTANCE TO POINT OF MAXIMUM CONCENTRATION. HEFFIV
C IS EFFECTIVE STACK HEIGHT (M).
C
  140 ACMAX=0.0
C
C PM IS MONTHLY PRECIPITATION IN CM/MON; CONVERT TO M/SEC.
C
  150 PM=HYDBAL(MON,2)*3.8580247E-9
C
C UWG IS WET DEPOSITION VELOCITY FOR GASES, ALWAYS NEEDED FOR
C VOLATILIZATION CALCULATIONS BELOW.
C
      UWG=WRATG*PM
      IF(AIRFLG.EQ.NONE)GO TO 225
      UD=UDG
      UWET=UWG
      IF(AIRPOL.EQ.GAS)GO TO 160
      UD=UDP
      UWET=WRATP*PM
  160 IF(AIRFLG.EQ.AREA)GO TO 225
C
C UD & UWET ARE DRY & WET DEPOSITION VELOCITIES FOR POLLUTANT FROM STACK
C
      UDPW=UD+UWET
C
C SET PARAMETERS FOR QUADRATURE ROUTINE D01AJF
C
      EPSREL=1.0E-4
      EPSABS=0.0
      ABSERR=0.0
      IFAIL=0
      HMIXZ=HMIX(MON,IYR)
      U=UW(MON,IYR)
      CALL D01AJF(DEPAVG,100.0,XMAX,EPSABS,EPSREL,DEPFAC,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL .NE. 0.
C
      IF(IFAIL.EQ.0)GO TO 170
      WRITE(IWP,165)IFAIL
 165  FORMAT(1X,'PROBLEM WITH D01AJF CALL IN AIR, QP CALCULATION, IFAIL
     $= ,'I3)
 170  CONTINUE
      VELFAC=-SQRT(2.0/PI)*UDPW/U
C
C QP IS DEPLETED SOURCE TERM AND IS USED BELOW.
C
      QP=QS(MON,IYR)*EXP(VELFAC*DEPFAC-AK*XMAX/U)
      SIGMAY=0.08*XMAX/SQRT(1.0+0.0001*XMAX)
      SIGMAZ=0.06*XMAX/SQRT(1.0+0.0015*XMAX)
      SIGZMX=2.0*(HMIXZ-HEFFIV)/2.15
C
C CHECK IF SIGZMX < 0.0 AND WRITE ERROR MESSAGE IF IT IS.
C
      IF(SIGZMX.GT.0.0)GO TO 190
      WRITE(IWP,175)MON,IYR
 175  FORMAT(1X,'ERROR IN AIR: MIXING HEIGHT .LT. EFFECTIVE STACK HEIGHT
     $ - SIGMA SUB Z .LT. 0.0 - INCREASE MIXYNG HEIGHT FOR MONTH',I3,
     $' YEAR',I3)
      STOP
 190  CONTINUE
      IF(SIGMAZ.GT.SIGZMX)SIGMAZ=SIGZMX
C
C COMPUTE MAXIMUM CONCENTRATION FOR POINT SOURCE
C
      ACMAX=QP*EXP(-0.5*((HEFFIV-VG*XMAX/U)/SIGMAZ)**2)/
     $      (PI*SIGMAY*SIGMAZ*U)
 225  IF(WATBOD.EQ.NO)GO TO 700
C
C
      IF(LAKE.NE.YES)GO TO 250
C
C  CALCULATE CONCENTRATION IN AIR FROM LAKE AND SOIL VOLATILIZATION
C
      IF(AIRFLG.EQ.AREA)ARL=(CTYLTH*CTYLTH-AREALK)*10000.0
C
C WAMOUL = WATER TO AIR VOLATILIZATION, SAMOUL = SOIL TO AIR VOLATILIZATION
C FOR LAKE.
C
      WSAMIN=WAMOUL+SAMOUL
      AREAT=AREALK+ARL*.0001
      DEDGE=0.5*SQRT(AREAT)
      C=SQRT(2.0/PI)*DEDGE**0.25/0.0375
      WSACON=C*WSAMIN/(AREAT*UW(MON,IYR))
      IF(AK.EQ.0.0)GO TO 230
      WSACON=WSACON*EXP(-DEDGE*AK/UW(MON,IYR))
 230  CONTINUE
C
C  CALCULATE WET (FWLAKE) & DRY (FDLAKE) DEPOSITION
C
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      ASMIDL=ASMODL
      ASMIWL=ASMOWL
      AWMINL=AWMOUL
      FDLAKE=WSACON*UDG
      FWLAKE=WSACON*UWG
      AWMOUL=FDLAKE+FWLAKE
C
C DEPOSITION RATE INTO LAKE AND ONTO SOIL ARE THE SAME; HOWEVER
C THE AREAS THIS RATE GOES INTO ARE DIFFERENT
C
      ASMODL=FDLAKE
      ASMOWL=FWLAKE
      IF(ARL.NE.0.0)GO TO 231
      ASMODL=0.
      ASMOWL=0.
 231  CONTINUE
C
      AWMOUL=AWMOUL*AREALK
      IF(AIRFLG.EQ.NONE)GO TO 243
      IF(AIRFLG.EQ.AREA)GO TO 240
      AROLD=ARL*0.0001
      ARL=AREASL*10000.0
C
C  ARL IS PLUME SURFACE AREA OVER SOIL NEXT TO LAKE (IN CM**2) TO BE
C  TRANSFERRED TO SESOIL.
C
      IF(ACMAX.EQ.0.0) GO TO 245
      IF(ISTEP.GT.1) GO TO 236
C
C CONST = 2.0*0.08 ; CALCULATION OF AREAS BELOW INCLUDES 2 SIGMAY'S
C ON EITHER SIDE OF PLUME CENTERLINE.
C
      CONST=0.16
C
C CALCULATE SIGMA SUB Y'S
C
      SIGY1=CONST*XMAX/SQRT(1.0+0.0001*XMAX)
      WLENL=SQRT(AREALK)
      XMXPLK=XMAX+WLENL
      SIGY2=CONST*XMXPLK/SQRT(1.0+0.0001*XMXPLK)
      XMXPLS=XMXPLK+XSOIL
      SIGY3=CONST*XMXPLS/SQRT(1.0+0.0001*XMXPLS)
C
C FIND AREA OF PLUME OVER LAKE AREAPL AND SOIL AREAPS USING
C TWO TRAPEZOIDS FOR EACH.
C
      AREAPL=(SIGY1+SIGY2)*WLENL
      AREAPS=(SIGY2+SIGY3)*XSOIL
      ARPLLK=AREALK
      IF(AREAPL.LE.AREALK) ARPLLK=AREAPL
      IF(AREAPL.GT.AREALK) AREAPS=AREAPS+(AREAPL-AREALK)
      AREASL=AREAPS
C
C CALCULATE CONCENTRATIONS AND DEPOSITIONS DUE TO AIR POINT SOURCE
C
      IFAIL=0
```

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C
C CALCULATE AVERAGE CONCENTRATION OVER LAKE AVCONL FROM POINT SOURCE
C 1ST FIND DEPLETION FACTOR (DEPFAC) FROM XMAX TO XMXPLK
C
      CALL D01AJF(DEPAVG,XMAX,XMXPLK,EPSABS,EPSREL,DEPFAC,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 265
      WRITE(IWP,260)IFAIL
 260  FORMAT(1X,'PROBLEM WITH D01AJF CALL IN AIR, LAKE SECTION, IFAIL =
     $',I3)
      STOP
 265  CONTINUE
      IFAIL=0
      CALL D01AJF(CAVGE,XMAX,XMXPLK,EPSABS,EPSREL,RESULT,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 275
      WRITE(IWP,260)IFAIL
      STOP
 275  CONTINUE
C
      AVCONL=QP*RESULT/WLENL
C
C CALCULATE AVERAGE CONCENTRATION OVER SOIL AVCONS
C 1ST, DEPLETE SOURCE QS FROM 0 TO XMXPLK
C
      IFAIL=0
      CALL D01AJF(DEPAVG,100.,XMXPLK,EPSABS,EPSREL,DEPFAC,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 280
      WRITE(IWP,260)IFAIL
      STOP
 280  CONTINUE
      QPS=QS(MON,IYR)*EXP(VELFAC*DEPFAC-AK*XMAX/U)
C
C CALCULATE DEPLETION FACTOR FROM XMXPLK TO XMXPLS
C
      IFAIL=0
      CALL D01AJF(DEPAVG,XMXPLK,XMXPLS,EPSABS,EPSREL,DEPFAC,ABSERR,
     $ WORK,800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 290
      WRITE(IWP,260)IFAIL
      STOP
 290  CONTINUE
      IFAIL=0
      CALL D01AJF(CAVGE,XMXPLK,XMXPLS,EPSABS,EPSREL,RESULT,ABSERR,
     $ WORK,800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 295
      WRITE(IWP,260)IFAIL
      STOP
 295  CONTINUE
      AVCONS=QPS*RESULT/XSOIL
      AVCSL=(AVCONS+AVCONL)/2.0
      SLAREA=AREAPS+ARPLLK
C
 236  CONTINUE
C
C CALCULATE DRY & WET DEPOSITION INTO LAKE DUE TO AIR POINT SOURCE
C  IN (KG/M**2/SEC)
C
      FDLAKE=AVCONL*UD
      FWLAKE=AVCONL*UWET
C
C CALCULATE TOTAL DEPOSITION IN LAKE IN (KG/SEC)
C
      AWMOUL=AWMOUL+(FDLAKE+FWLAKE)*ARPLLK
C
C CALCULATE DEPOSITION ONTO SOIL DUE TO AIR POINT SOURCE
C
      FDSOIL=AVCONS*UD
      FWSOIL=AVCONS*UWET
C
C DEPOSITION DUE TO VOLATILIZATION CONCENTRATION ABOVE MUST GO INTO
C  SOIL AREA (AREASL). VALUES IN KG/M**2/SEC
C
      ASMODL=ASMODL*AROLD/AREASL+FDSOIL
      ASMOWL=ASMOWL*AROLD/AREASL+FWSOIL
      GO TO 245
C
C CALCULATE DEPOSITION DUE TO AREA SOURCE
C
 240  FDLAKE=ACMAX*UD
      FWLAKE=ACMAX*UWET
      AWMOUL=AWMOUL+AREALK*(FDLAKE+FWLAKE)
C
C DEPOSITION FOR SOIL SAME AS FOR LAKE(AREA DIFFERENT HOWEVER)
C
      ASMODL=ASMODL+FDLAKE
      ASMOWL=ASMOWL+FWLAKE
      AREASL=ARL*.0001
      AVCSL=ACMAX
      SLAREA=CTYLTH*CTYLTH
      GO TO 245
 243  AVCSL=0.0
      SLAREA=0.0
 245  IF(ISTEP.GT.1)GO TO 247
      ASDEPL=0.0
      AWDEPL=0.0
```

```
C
C ASDEPL & AWDEPL (TOTAL DEPOSITION TO SOIL AND WATER - LAKE) CONVERTED
C  TO UG FROM KG
C
 247  ASDEPL=ASDEPL+(ASMODL+ASMOWL)*AREASL*DT*1.0E+9
      AWDEPL=AWDEPL+AWMOUL*DT*1.0E+9
      IF(ISTEP.LT.NSTEPS)GO TO 250
C
C CALCULATE AVERAGE AIR CONCENTRATION AVAIRL FOR LAKE
C
      AVAIRL=(AVCSL*SLAREA+WSACON*AREAT)/AMAX1(AREAT,SLAREA)
C
C CONVERT FROM KG/M**3 TO UG/M**3
C
      AVAIRL=AVAIRL*1.0E+9
      IF(AIRFLG.NE.AREA)ACMAXL=(WSACON+ACMAX)*1.0E+9
C
C
 250  IF(RIVER.NE.YES)GO TO 400
C
C  CALCULATE CONCENTRATION IN AIR FROM RIVER VOLATILIZATION
C
      WAMINR=0
      DO 325 I=1,NR
 325  WAMINR=WAMINR+WAMOUR(I)
C
C WAMINR IS TOTAL KG/SEC COMING FROM RIVER DUE TO VOLATILIZATION
C
      AREARE=WWIDR*WLENR
C
C AREAR IS TOTAL SURFACE AREA OF RIVER
C
      AREAR=AREARE*FLOAT(NR)
      IF(AIRFLG.EQ.AREA)ARR=(CTYLTH*CTYLTH-AREAR)*10000.
      AREAT=AREAR+ARR*.0001
C
C WSAMIN IS TOTAL KG/SEC COMING FROM RIVER AND SOIL DUE
C   TO VOLATILIZATION (ARR INITIALIZED AS GEOM(1))
C
      WSAMIN=WAMINR+SAMOUR
      DEDGE=0.5*SQRT(AREAT)
      C=SQRT(2.0/PI)*DEDGE**0.25/0.0375
      WSACON=C*WSAMIN/(AREAT*UW(MON,IYR))
      IF(AK.EQ.0.0) GO TO 350
      WSACON=WSACON*EXP(-DEDGE*AK/UW(MON,IYR))
 350  CONTINUE
C
C CALCULATE WET (FWRIV) & DRY (FDRIV) DEPOSITION DUE
C TO CONCENTRATION CALCULATED FROM VOLATILIZATION.
C
      AWMINR=AWMOUR
      ASMIDR=ASMODR
      ASMIWR=ASMOWR
      FDRIV=WSACON*UDG
      FWRIV=WSACON*UWG
      AWMOUR=FDRIV+FWRIV
```

```
C
C DEPOSITION RATE INTO RIVER AND ONTO SOIL ARE SAME; HOWEVER,
C   THE AREAS THIS RATE GOES INTO ARE DIFFERENT.
C
      ASMODR=FDRIV
      ASMOWR=FWRIV
      IF(ARR.NE.0.0)GO TO 360
      ASMODR=0.
      ASMOWR=0.
 360  CONTINUE
      AWMOUR=AWMOUR*AREARE
      IF(AIRFLG.EQ.NONE) GO TO 397
      IF(AIRFLG.EQ.AREA) GO TO 396
      AROLD=ARR*.0001
      ARR=AREASR*10000.
C
C  ARR IS PLUME SURFACE AREA OVER SOIL NEXT TO RIVER (IN CM**2) TO BE
C  TRANSFERRED TO SESOIL.
C
      IF(ACMAX.EQ.0.0) GO TO 398
      IF(ISTEP.GT.1) GO TO 395
      ARRTPS=1.0
C
C CONST = 2.0*0.08 ; CALCULATION OF AREAS BELOW INCLUDES 2 SIGMAY'S ON
C EITHER SIDE OF PLUME CENTERLINE
C
      CONST=0.16
C
C CALCULATE SIGMA SUB Y'S
C
      SIGY1=CONST*XMAX/SQRT(1.0+0.0001*XMAX)
      TWLENR=FLOAT(NR)*WLENR
      XMAXPR=XMAX+TWLENR
      SIGY2=CONST*XMAXPR/SQRT(1.0+0.0001*XMAXPR)
C
C FIND AREA OF PLUME OVER RIVER AND SOIL USING TRAPEZOID
C
      ARPLSR=(SIGY1+SIGY2)*TWLENR
      ARPLR=AREAR
      IF(ARPLSR.LE.AREAR) GO TO 385
C
C CALCULATE AREA OF PLUME OVER SOIL (AREAPS)
C
      AREAPS=ARPLSR-AREAR
      AREASR=AREAPS
      GO TO 390
 385  ARRTPS=0.0
      ARPLR=ARPLSR
      AREASR=AROLD
 390  CONTINUE
C
C CALCULATE AVERAGE CONCENTRATION & DEPOSITIONS DUE TO AIR POINT SOURCE
C FOR RIVER
C
      IFAIL=0
C
```

```
C 1ST,FIND DEPLETION FACTOR (DEPFAC) FROM XMAX TO XMAXPR
C
      CALL D01AJF(DEPAVG,XMAX,XMAXPR,EPSABS,EPSREL,DEPFAC,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 370
      WRITE(IWP,365)IFAIL
  365 FORMAT(1X,'PROBLEM WITH D01AJF CALL IN AIR, RIVER SECTION, IFAIL =
     $ ',I3)
      STOP
  370 CONTINUE
      IFAIL=0
      CALL D01AJF(CAVGE,XMAX,XMAXPR,EPSABS,EPSREL,RESULT,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 375
      WRITE(IWP,365)IFAIL
      STOP
  375 CONTINUE
C
C CALCULATE AVERAGE CONCENTRATION OVER RIVER AND SOIL NEXT TO RIVER
C
      AVCNRS=QP*RESULT/TWLENR
  395 CONTINUE
C
C CALCULATE DRY AND WET DEPOSITION INTO RIVER DUE TO POINT SOURCE
C  IN KG/M**2/SEC
C
      FDRIV=AVCNRS*UD
      FWRIV=AVCNRS*UWET
C
C CALCULATE TOTAL DEPOSITION INTO EACH REACH IN KG/SEC
C
      AWMOUR=AWMOUR+(FDRIV+FWRIV)*ARPLR/FLOAT(NR)
C
C CALCULATE DEPOSITION ONTO SOIL NEXT TO RIVER DUE TO POINT SOURCE
C
      IF(AREASR.EQ.0.0)GO TO 398
      FDSOIL=AVCNRS*UD
      FWSOIL=AVCNRS*UWET
C
C DEPOSITION DUE TO VOLATILIZATION CONCENTRATION ABOVE MUST
C   GO INTO SOIL AREA AREASR; VALUES ARE IN KG/M**2/SEC
C
      ASMODR=ASMODR*AROLD/AREASR+FDSOIL*ARRTPS
      ASMOWR=ASMOWR*AROLD/AREASR+FWSOIL*ARRTPS
      GO TO 398
C
C CALCULATE DEPOSITION DUE TO AREA SOURCE
C
  396 FDRIV=ACMAX*UD
      FWRIV=ACMAX*UWET
      AWMOUR=AWMOUR+AREARE*(FDRIV+FWRIV)
C
C DEPOSITION FOR SOIL SAME AS FOR RIVER (AREAS DIFFERENT HOWEVER)
C
      ASMODR=ASMODR+FDRIV
      ASMOWR=ASMOWR+FWRIV
      AREASR=ARR*.0001
      AVCNRS=ACMAX
      ARPLSR=CTYLTH*CTYLTH
      GO TO 398
 397  AVCNRS=0.0
      ARPLSR=0.0
 398  IF(ISTEP.GT.1)GO TO 399
      ASDEPR=0.0
      AWDEPR=0.0
C
C CALCULATE TOTAL MONTHLY DEPOSITION IN UG ONTO SOIL (ASDEPR) &
C INTO WATER (AWDEPR) FOR RIVER
C
 399  ASDEPR=ASDEPR+(ASMODR+ASMOWR)*AREASR*DT*1.0E+9
      AWDEPR=AWDEPR+AWMOUR*DT*1.0E+9*FLOAT(MR)
      IF(ISTEP.LT.NSTEPS) GO TO 400
C
C CALCULATE AVERAGE & MAXIMUM AIR CONCENTRATION IN UG/M**3
C
      AVAIRR=(WSACON*AREAT+AVCNRS*ARPLSR)/AMAX1(AREAT,ARPLSR)
      AVAIRR=AVAIRR*1.0E+9
      IF(AIRFLG.NE.AREA)ACMAXR=(ACMAX+WSACON)*1.0E+9
C
C
 400  IF(ESTU.NE.YES)RETURN
C
C  CALCULATE CONCENTRATION IN AIR FROM ESTUARY VOLATILIZATION
C
      AREAE=WLENE*WWIDE
      IF(AIRFLG.EQ.AREA) ARE=(CTYLTH*CTYLTH-AREAE)*10000.0
      AREAT=AREAE+ARE*.0001
      WSAMIN=WAMOUE+SAMOUE
      DEDGE=0.5*SQRT(AREAT)
      C=SQRT(2.0/PI)*DEDGE**0.25/0.0375
      WSACON=C*WSAMIN/(AREAT*UW(MON,IYR))
      IF(AK.EQ.0.0)GO TO 425
      WSACON=WSACON*EXP(-DEDGE*AK/UW(MON,IYR))
 425  CONTINUE
C
C  CALCULATE WET (FWEST) & DRY (FDEST) DEPOSITION
C
      AWMINE=AWMOUE
      ASMIDE=ASMODE
      ASMIWE=ASMOWE
      FDEST=WSACON*UDG
      FWEST=WSACON*UWG
      AWMOUE=FDEST+FWEST
C
C DEPOSITION RATE INTO ESTUARY AND ONTO SOIL ARE SAME; HOWEVER,
C   THE AREAS THIS RATE GOES INTO ARE DIFFERENT
```

```
C
      ASMODE=FDEST
      ASMOWE=FWEST
      IF(ARE.NE.0.0)GO TO 427
      ASMODE=0.
      ASMOWE=0.
 427  CONTINUE
      AWMOUE=AWMOUE*AREAE
      IF(AIRFLG.EQ.NONE) GO TO 453
      IF(AIRFLG.EQ.AREA) GO TO 450
      AROLD=ARE*.0001
      ARE=AREASE*10000.
C
C  ARE IS PLUME SURFACE AREA OVER SOIL NEXT TO ESTUARY (IN CM**2) TO BE
C  TRANSFERRED TO SESOIL
C
      IF(ACMAX.EQ.0.0) GO TO 455
      IF(ISTEP.GT.1) GO TO 445
      AERTPS=1.0
C
C CONST = 2.0*0.08 ; CALCULATIONS OF AREAS BELOW INCLUDES 2 SIGMAY'S ON
C EITHER SIDE OF PLUME CENTERLINE
C
      CONST=0.16
C
C CALCULATE SIGMA SUB Y'S
C
      SIGY1=CONST*XMAX/SQRT(1.0+0.0001*XMAX)
      XMAXPE=XMAX+WLENE
      SIGY2=CONST*XMAXPE/SQRT(1.0+0.0001*XMAXPE)
C
C FIND AREA OF PLUME OVER ESTUARY AND SOIL USING TRAPEZOID
C
      ARPLSE=(SIGY1+SIGY2)*WLENE
      ARPLE=AREAE
      IF(ARPLSE.LE.AREAE) GO TO 435
C
C CALCULATE AREA OF PLUME OVER SOIL (AREAPS) NEXT TO ESTUARY
C
      AREAPS=ARPLSE-AREAE
      AREASE=AREAPS
      GO TO 440
 435  AERTPS=0.0
      ARPLE=ARPLSE
      AREASE=AROLD
 440  CONTINUE
C
C CALCULCATE AVERAGE CONCENTRATION & DEPOSITION DUE TO AIR POINT SOURCE
C
      IFAIL=0
C
C 1ST, FIND DEPLETION FACTOR (DEPFAC) FROM XMAX TO XMAXPE
C
      CALL D01AJF(DEPAVG,XMAX,XMAXPE,EPSABS,EPSREL,DEPFAC,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
```

```
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 485
      WRITE(IWP,480)IFAIL
 480  FORMAT(1X,'PROBLEM WITH D01AJF CALL IN AIR, ESTUARY SECTION, IFAIL
     $ = ',I3)
      STOP
 485  CONTINUE
      IFAIL=0
      CALL D01AJF(CAVGE,XMAX,XMAXPE,EPSABS,EPSREL,RESULT,ABSERR,WORK,
     $ 800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL NOT EQUAL TO 0
C
      IF(IFAIL.EQ.0)GO TO 490
      WRITE(IWP,480)IFAIL
      STOP
 490  CONTINUE
C
C CALCULATE AVERAGE CONCENTRATION OVER ESTUARY AND SOIL NEXT
C   TO ESTUARY
C
      AVCNES=QP*RESULT/WLENE
 445  CONTINUE
C
C CALCULATE DRY AND WET DEPOSITION INTO ESTUARY DUE TO
C   POINT SOURCE IN KG/M**2/SEC
C
      FDEST=AVCNES*UD
      FWEST=AVCNES*UWET
C
C CALCULATE TOTAL DEPOSITION INTO ESTUARY IN KG/SEC
C
      AWMOUE=AWMOUE+(FDEST+FWEST)*ARPLE
C
C CALCULATE DEPOSITION ONTO SOIL NEXT TO ESTUARY DUE TO
C   POINT SOURCE
C
      IF(AREASE.EQ.0.0)GO TO 455
      FDSOIL=AVCNES*UD
      FWSOIL=AVCNES*UWET
C
C DEPOSITION DUE TO VOLATILIZATION CONCENTRATION ABOVE MUST GO INTO
C  SOIL AREA AREASE; VALUES ARE IN KG/M**2/SEC
C
      ASMODE=ASMODE*AROLD/AREASE+FDSOIL*AERTPS
      ASMOWE=ASMOWE*AROLD/AREASE+FWSOIL*AERTPS
      GO TO 455
C
C CALCULATE DEPOSITION DUE TO AREA SOURCE
C
 450  FDEST=ACMAX*UD
      FWEST=ACMAX*UWET
      AWMOUE=AWMOUE+AREAE*(FDEST+FWEST)
C
C DEPOSITION FOR SOIL SAME AS FOR ESTUARY (AREAS DIFFERENT, HOWEVER)
```

```
C
      ASMODE=ASMODE+FDEST
      ASMOWE=ASMOWE+FWEST
      AREASE=ARE*.0001
      AVCNES=ACMAX
      ARPLSE=CTYLTH*CTYLTH
      GO TO 455
 453  AVCNES=0.
      ARPLSE=0.
 455  IF(ISTEP.GT.1)GO TO 475
      ASDEPE=0.0
      AWDEPE=0.0
C
C CALCULATE TOTAL MONTHLY DEPOSITION ONTO SOIL AND INTO ESTUARY IN UG
C
 475  ASDEPE=ASDEPE+(ASMODE+ASMOWE)*AREASE*DT*1.0E+9
      AWDEPE=AWDEPE+AWMOUE*DT*1.0E+9
      IF(ISTEP.LT.NSTEPS) RETURN
C
C CALCULATE AVERAGE & MAXIMUM AIR CONCENTRATION IN UG/M**3 (ABOVE
C ESTUARY)
C
      AVAIRE=(WSACON*AREAT+AVCNES*ARPLSE)/AMAX1(AREAT,ARPLSE)
      AVAIRE=1.0E+9*AVAIRE
      IF(AIRFLG.EQ.POINT)ACMAXE=(ACMAX+WSACON)*1.0E+9
      RETURN
C
C
C NO WATER BODY IS CONSIDERED; COMPUTE CONCENTRATION OF AIR OVER SOIL
C
 700  CONTINUE
      IF(AIRFLG.EQ.AREA)ARS=CTYLTH*CTYLTH*10000.0
      AREAT=ARS*0.0001
      IF(AREAT.EQ.0.0)GO TO 725
C
C COMPUTE CONCENTRATION IN AIR DUE TO VOLATILIZATION FROM SOIL
C
      SAMIN=SAMOUS
      DEDGE=0.5*SQRT(AREAT)
      C=SQRT(2.0/PI)*DEDGE**0.25/0.0375
      SACON=C*SAMIN/(AREAT*UW(MON,IYR))
      IF(AK.EQ.0.0)GO TO 725
      SACON=SACON*EXP(-DEDGE*AK/UW(MON,IYR))
      GO TO 730
 725  CONTINUE
      SACON=0.0
 730  ASMIDS=ASMODS
      ASMIWS=ASMOWS
C
C CALCULATE DRY & WET DEPOSITION ONTO SOIL DUE TO CONCENTRATION FROM
C VOLATILIZATION
C
      ASMODS=SACON*UDG
      ASMOWS=SACON*UWG
      IF(AIRFLG.EQ.NONE)GO TO 753
      IF(AIRFLG.EQ.AREA)GO TO 750
      AROLD=ARS*0.0001
      ARS=AREAS*10000.
      IF(ACMAX.EQ.0.0)GO TO 755
      IF(ISTEP.GT.1)GO TO 745
C
C CONST=2.0*0.08 ; CALCULATION OF AREAS BELOW INCLUDES 2 SIGMAY'S
C ON EITHER SIDE OF PLUME CENTERLINE
C
      CONST=0.16
C
C CALCULATE SIGMA SUB Y'S
C
      SIGY1=CONST*XMAX/SQRT(1.0+0.0001*XMAX)
      XMAXPS=XMAX+XLENS
      SIGY2=CONST*XMAXPS/SQRT(1.0+0.0001*XMAXPS)
C
C FIND AREA OF PLUME OVER SOIL USING TRAPEZOID
C
      ARPLS=(SIGY1+SIGY2)*XLENS
      AREAS=ARPLS
C
C CALCULATE AVERAGE CONCENTRATION & DEPOSITION DUE TO AIR POINT SOURCE
C
      IFAIL=0
C
C 1ST, FIND DEPLETION FACTOR (DEPFAC) FROM XMAX TO XMAXPS
C
      CALL D01AJF(DEPAVG,XMAX,XMAXPS,EPSABS,EPSREL,DEPFAC,ABSERR,
     $ WORK,800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL .NE. 0
C
      IF(IFAIL.EQ.0)GO TO 735
      WRITE(IWP,732)IFAIL
 732  FORMAT(1X,'PROBLEM WITH D01AJF CALL IN AIR, SOIL SECTION, IFAIL =
     $',I3)
      STOP
 735  CONTINUE
      IFAIL=0
      CALL D01AJF(CAVGE,XMAX,XMAXPS,EPSABS,EPSREL,RESULT,ABSERR,
     $ WORK,800,IWORK,102,IFAIL)
C
C WRITE ERROR MESSAGE IF IFAIL .NE. 0
C
      IF(IFAIL.EQ.0)GO TO 740
      WRITE(IWP,732)
      STOP
 740  CONTINUE
C
C CALCULATE AVERAGE CONCENTRATION IN AIR OVER SOIL AVCNS
C
      AVCNS=QP*RESULT/XLENS
 745  CONTINUE
C
C CALCULATE DRY & WET DEPOSITION ONTO SOIL DUE TO POINT SOURCE
C IN KG/M**2/S
```

```
C
      FDSOIL=AVCNS*UD
      FWSOIL=AVCNS*UWET
C
C DEPOSITION DUE TO VOLATILIZATION CONCENTRATION ABOVE MUST GO INTO
C SOIL AREA AREAS; VALUES ARE IN KG/M**2/S
C
      ASMODS=ASMODS*AROLD/AREAS+FDSOIL
      ASMOWS=ASMOWS*AROLD/AREAS+FWSOIL
      GO TO 755
C
C CALCULATE DEPOSITION DUE TO AREA SOURCE
C
 750  FDSOIL=ACMAX*UD
      FWSOIL=ACMAX*UWET
      ASMODS=ASMODS+FDSOIL
      ASMOWS=ASMOWS+FWSOIL
      AREAS=ARS*.0001
      AVCNS=ACMAX
      ARPLS=CTYLTH*CTYLTH
      GO TO 755
 753  AVCNS=0.
      ARPLS=0.
 755  IF(ISTEP.GT.1)GO TO 775
      ASDEPS=0.0
C
C CALCULATE TOTAL MONTHLY DEPOSITION ONTO SOIL IN UG
C
 775  ASDEPS=ASDEPS+(ASMODS+ASMOWS)*AREAS*DT*1.0E+9
      IF(ISTEP.LT.NSTEPS)RETURN
C
C CALCULATE AVERAGE & MAXIMUM AIR CONCENTRATION ABOVE SOIL IN UG/M**3
C
      AVAIRS=(SACON*AREAT+AVCNS*ARPLS)/AMAX1(AREAT,ARPLS)
      AVAIRS=1.0E+9*AVAIRS
      IF(AIRFLG.NE.AREA)ACMAXS=(SACON+ACMAX)*1.0E+9
      RETURN
      END
      SUBROUTINE ALPHA(IMON,IYR)
      COMMON/SDPARE/SEDCE(12,10),CONSDE
      COMMON/SDPARO/SEDCO(12,10),CONSDO
      COMMON/SDPARR/SEDCR(12,10),DIASDR,DENSDR,DENWR,SLOPER,CONSDR
      COMMON/SDPARL/SEDCL(12,10),DIASDT,DENSDT,DENWT,SLOPET,WDEPT,CONSDL
      COMMON/EQUIL/DISK,HPLUSL,HPLUSR,HPLUSE,HPLUSO,
     $                  SWKSWL,SWKSWR,SWKSWE,SWKSWO
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $             ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/ALPHAS/A1L,A2L,A3L,A1R,A2R,A3R,A1E,A2E,A3E,
     $              A1O,A2O,A3O
      REAL LAKE
      DATA YES/4H YES/,EPS/1.0E-5/,BASE/4HBASE/,IDENOM/1/,NONE/4HNONE/
      IWP=13
      MON=IMON
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 50
      IF(CHMFLG.EQ.BASE.AND.DISK.EQ.0.0)IDENOM=0
C
C
 50   IF(LAKE.NE.YES)GO TO 100
      IF(IDENOM.EQ.0)GO TO 75
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 70
C
C COMPUTE DISSOCIATION CONSTANT OVER H-PLUS (DISOHL) TO BE USED BELOW.
C
      IF(CHMFLG.EQ.NONE)GO TO 60
C
C IF CHMFLG IS BASE THEN CONVERT HPLUS TO [OH-]
C
      IF(CHMFLG.EQ.BASE)HPLUSL=1.0E-14/HPLUSL
      DISOHL=DISK/HPLUSL
      IF(CHMFLG.EQ.BASE)DISOHL=1.0/DISOHL
      DISP1L=DISOHL+1.0
      GO TO 70
 60   DISP1L=1.0
      DISOHL=0.0
 70   CONTINUE
C
C CONSDL IS IN KG/M**3; NEED KG/L HERE, SO MULTIPLY BY 0.001.
C COMPUTE ADSORPTION TERM (ADSORB) AND DENOMINATOR (DENOM)
C
      ADSORB=SWKSWL*CONSDL*.001
      DENOM=DISP1L+ADSORB
C
C CALCULATE ALPHA 1 & 2 & 3 FOR LAKE.
C
      A1L=1.0/DENOM
      A2L=DISOHL/DENOM
      A3L=ADSORB/DENOM
      GO TO 80
 75   A1L=0.0
      A2L=1.0
      A3L=0.0
 80   CONTINUE
      IF((A1L+A2L+A3L-1.0).LT.EPS)GO TO 100
C
```

```
C WRITE ERROR MESSAGE
C
      WRITE(IWP,90)
 90   FORMAT(1X,'ERROR IN ALPHA ROUTINE, ALPHAS FOR LAKE DO NOT ADD UP T
     $O 1.0')
      STOP
C
C
 100  IF(RIVER.NE.YES)GO TO 200
      IF(IDENOM.EQ.0)GO TO 150
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 170
C
C COMPUTE DISSOCIATION CONSTANT OVER H-PLUS (DISOHR) TO BE USED BELOW.
C
      IF(CHMFLG.EQ.NONE)GO TO 160
C
C IF CHMFLG IS BASE THEN CONVERT HPLUS TO [OH-]
C
      IF(CHMFLG.EQ.BASE)HPLUSR=1.0E-14/HPLUSR
      DISOHR=DISK/HPLUSR
      IF(CHMFLG.EQ.BASE)DISOHR=1.0/DISOHR
      DISP1R=DISOHR+1.0
      GO TO 170
 160  DISP1R=1.0
      DISOHR=0.0
 170  CONTINUE
C
C CONSDR IS IN KG/M**3, NEED KG/L, SO MULTIPLY BY .001
C COMPUTE ADSORPTION TERM (ADSORB) AND DENOMINATOR (DENOM)
C
      ADSORB=SWKSWR*CONSDR*.001
      DENOM=DISP1R+ADSORB
C
C COMPUTE ALPHA 1 & 2 & 3 FOR RIVER.
C
      A1R=1.0/DENOM
      A2R=DISOHR/DENOM
      A3R=ADSORB/DENOM
      GO TO 175
 150  A1R=0.
      A2R=1.
      A3R=0.
 175  CONTINUE
      IF((A1R+A2R+A3R-1.0).LT.EPS)GO TO 200
C
C WRITE ERROR MESSAGE
C
      WRITE(IWP,180)
 180  FORMAT(1X,'ERROR IN ALPHA ROUTINE, ALPHAS FOR RIVER DO NOT ADD UP
     $TO 1.0')
      STOP
C
C
 200  IF(ESTU.NE.YES)GO TO 300
      IF(IDENOM.EQ.0)GO TO 250
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 270
```

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C
C COMPUTE DISSOCIATION CONSTANT OVER H-PLUS (DISOHE) TO BE USED BELOW.
C
      IF(CHMFLG.EQ.NONE)GO TO 260
C
C IF CHMFLG IS BASE THEN CONVERT HPLUS TO [OH-]
C
      IF(CHMFLG.EQ.BASE)HPLUSE=1.0E-14/HPLUSE
      DISOHE=DISK/HPLUSE
      IF(CHMFLG.EQ.BASE)DISOHE=1.0/DISOHE
      DISP1E=DISOHE+1.0
      GO TO 270
 260  DISP1E=1.0
      DISOHE=0.0
 270  CONTINUE
C
C CONSDE IS IN KG/M**3, NEED KG/L HERE, SO MULTIPLY BY .001
C COMPUTE ADSORPTION TERM (ADSORB) AND DENOMINATOR (DENOM)
C
      ADSORB=SWKSWE*CONSDE*.001
      DENOM=DISP1E+ADSORB
C
C COMPUTE ALPHA 1 & 2 & 3 FOR ESTUARY
C
      A1E=1.0/DENOM
      A2E=DISOHE/DENOM
      A3E=ADSORB/DENOM
      GO TO 275
 250  A1E=0.
      A2E=1.
      A3E=0.
 275  CONTINUE
      IF((A1E+A2E+A3E-1.0).LT.EPS)GO TO 300
C
C WRITE ERROR MESSAGE
C
      WRITE(IWP,280)
 280  FORMAT(1X,'ERROR IN ALPHA ROUTINE, ALPHAS FOR ESTUARY DO NOT ADD U
     $P TO 1.0')
      STOP
C
C
 300  IF(OCEAN.NE.YES)RETURN
      IF(IDENOM.EQ.0)GO TO 350
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 370
C
C COMPUTE DISSOCIATION CONSTANT OVER H-PLUS (DISOHO) TO BE USED BELOW.
C
      IF(CHMFLG.EQ.NONE)GO TO 360
C
C IF CHMFLG IS BASE THEN CONVERT HPLUS TO [OH-]
C
      IF(CHMFLG.EQ.BASE)HPLUSO=1.0E-14/HPLUSO
      DISOHO=DISK/HPLUSO
      IF(CHMFLG.EQ.BASE)DISOHO=1.0/DISOHO
      DISP1O=DISOHO+1.0
      GO TO 370
 360  DISP1O=1.0
      DISOHO=0.0
 370  CONTINUE
C
C CONSDO IS IN KG/M**3, NEED KG/L HERE, SO MULTIPLY BY .001
C COMPUTE ADSORPTION TERM (ADSORB) AND DENOMINATOR (DENOM)
C
      ADSORB=SWKSWO*CONSDO*.001
      DENOM=DISP1O+ADSORB
C
C COMPUTE ALPHA 1 & 2 & 3 FOR OCEAN
C
      A1O=1.0/DENOM
      A2O=DISOHO/DENOM
      A3O=ADSORB/DENOM
      GO TO 375
 350  A1O=0.
      A2O=1.
      A3O=0.
 375  CONTINUE
      IF((A1O+A2O+A3O-1.0).LT.EPS)RETURN
C
C WRITE ERROR MESSAGE
C
      WRITE(IWP,380)
 380  FORMAT(1X,'ERROR IN ALPHA ROUTINE, ALPHAS FOR OCEAN DO NOT ADD UP
     $TO 1.0')
      STOP
      END
      SUBROUTINE BIOCHN(IMO,IYR)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $             ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/WPARR/WVELR(12,10),WMINR(12,10),WMTRIV(20),
     $             NR,WWIDR,WLENR,WDEPR,WVOLR,WMTOLD,AREAR
      COMMON/WPARE/WVELE(12,10),WMINE(12,10),TIDMAX,EL,WWIDE,
     $             WLENE,WDEPE,NPTSE,AREAE
      COMMON/WPARO/WVELO(12,10),WCINO(12,10),BO,XOCEAN,NPTSO
      COMMON/SPARS/ARS,AREAS,XLENS
      COMMON/SPARL/ARL,AREASL,XSOIL
      COMMON/SPARR/ARR,AREASR
      COMMON/SPARE/ARE,AREASE
      COMMON/OUT/ACMAXL,AVAIRL,AVAIRR,AVAIRE,AWDEPL,AWDEPR,AWDEPE,
     $           ASDEPL,ASDEPR,ASDEPE,WVOLAL,WVOLAR,WVOLAE,SVOLAL,
     $           SVOLAR,SVOLAE,SWSURL,SWSURR,SWSURE,SWGRWL,SWGRWR,
     $           SWGRWE,SCONUL,SCONUR,SCONUE,SCONLL,SCONLR,SCONLE,
     $           CONL1,CONL2,CONL3,CONR1(20),CONR2(20),CONR3(20),
     $           CNCED1(11),CNCED2(11),CNCED3(11),CNCEU1(11),CNCEU2(11),
     $           CNCEU3(11),XESTY(11),CONO1(10),CONO2(10),CONO3(10),
     $           RESUSE,WASHL,WASHR,WASHE,ACMAXR,ACMAXE,ACMAXS,
     $           AVAIRS,ASDEPS,SVOLAS,SWGRWS,SCONUS,SCONLS,RESUSS,
     $           RESUSL,RESUSR,SCONML,SCONMR,SCONME,SCONMS,SWSURS,
     $           WASHS,AREA1(3)
      REAL KOW,LAMBDA,NO,KD,KOC,LOGKOW,LAKE
      DIMENSION AMO(12)
      DATA AMO/' OCT',' NOV',' DEC',' JAN',' FEB',' MAR',
     $' APR',' MAY',' JUN',' JUL',' AUG',' SEP'/
      DATA YES/' YES'/,NO/'  NO'/
      IF(IMO.NE.1.OR.IYR.GT.1)GO TO 280
      IRB=18
      IWB=19
      READ(IRB,10)COVFLG
 10   FORMAT(A4)
      WRITE(IWB,20)
 20   FORMAT('1',44X,'FOOD CHAIN BIOACCUMULATION FLAG')
      WRITE(IWB,30)
 30   FORMAT('0',26X,'OPTION CHOSEN',6X,'NAME',21X,'MEANING',/)
      IF(COVFLG.EQ.YES)GO TO 70
      IF(COVFLG.NE.NO)GO TO 50
      WRITE(IWB,40)
 40   FORMAT(38X,'NO',5X,'COVFLG',5X,'SIGNIFIES COMPOUND IS NOT A COVALE
     $NTLY BONDING MATERIAL')
      GO TO 100
 50   WRITE(IWB,60)COVFLG
 60   FORMAT(1X,'ERROR IN DATA: COVFLG DOES NOT EQUAL YES OR NO, BUT = '
     $,A4)
      STOP
 70   WRITE(IWB,80)
 80   FORMAT(37X,'YES',5X,'COVFLG',5X,'SIGNIFIES COMPOUND IS A COVALENTL
     $Y BONDING MATERIAL',///)
      WRITE(IWB,90)
 90   FORMAT(37X,'BIOACCUMULATION CANNOT BE ESTIMATED BY THE EMPLOYED ME
     $THOD')
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```
      RETURN
  100 CONTINUE
C
C     INITIALIZE CONCENTRATION VARIABLES FOR AQUATIC & PLANT PHASES FOR
C     LAKE, RIVER, ESTUARY, OCEAN, & SOIL-AIR OPTION.
C
      CONAQL=0.
      CONPLL=0.
      CONPLR=0.
      CONAQR=0.
      CONPLE=0.
      CONAQE=0.
      CONAQO=0.
      CONPLS=0.
      READ(IRB,110)KOW,R,YV,LAMBDA,TE
  110 FORMAT(20X,6E10.3)
      WRITE(IWB,120)
  120 FORMAT('0',////,42X,'FOOD CHAIN BIOACCUMULATION PARAMETERS')
      WRITE(IWB,130)
  130 FORMAT('0',30X,'DEFINITION',20X,'NAME',9X,'UNIT',6X,'VALUE',/)
      WRITE(IWB,140)KOW
  140 FORMAT(19X,'N-OCTANOL WATER PARTITION COEFFICIENT',6X,'KOW',9X,'(-
     $)',4X,1PE10.3)
      IF(OCEAN.EQ.YES.AND.LAKE.EQ.NO.AND.RIVER.EQ.NO.AND.ESTU.EQ.NO)
     $    GO TO 205
      WRITE(IWB,150)R
  150 FORMAT(27X,'INITIAL INTERCEPTION FRACTION',7X,'R',10X,'(-)',4X,
     $1PE10.3)
      WRITE(IWB,160)YV
  160 FORMAT(37X,'FORAGE PRODUCTIVITY',6X,'YV',9X,'G/M**2',2X,1PE10.3)
      WRITE(IWB,170)LAMBDA
  170 FORMAT(37X,'WEATHERING CONSTANT',4X,'LAMBDA',6X,'DAY**-1',2X,
     $1PE10.3)
      WRITE(IWB,180)TE
  180 FORMAT(18X,'GROWTH PERIOD OF FORAGE BEFORE HARVEST',6X,'TE',10X,
     $'DAY',4X,1PE10.3)
C
C     COMPUTE SOIL DENSITY RS IN G/M**3 (RS IS INPUT IN G/CM**3)
C
      RS=SOIL1(1)*1.0E+6
      KD=CHEM1(6)
      IF(KD.NE.0.)GO TO 190
      KOC=CHEM1(2)
      OC=SOIL1(5)
      KD=KOC*OC/100.
  190 WRITE(IWB,200)KD
  200 FORMAT(24X,'SOIL WATER PARTITION COEFFICIENT',6X,'KD',10X,'(-)',
     $4X,1PE10.3)
  205 WRITE(IWB,210)
  210 FORMAT(/////,49X,'BIOACCUMULATION FACTORS: ')
      IF(WATBOD.EQ.NO)GO TO 225
      BCFAQ=0.048*KOW
      WRITE(IWB,220)BCFAQ
  220 FORMAT('0',23X,'BCFAQ (AQUATIC) = CONC. IN TISSUE (FRESH WT.)/CONC
     $. IN WATER  (ML/G) = ',1PE10.3)
      IF(OCEAN.EQ.YES.AND.LAKE.EQ.NO.AND.RIVER.EQ.NO.AND.ESTU.EQ.NO)
     $GO TO 273
  225 BCFPL=EXP((ALOG(KD)-3.02)/(-0.85))
      WRITE(IWB,230)BCFPL
  230 FORMAT(24X,'BCFPL (PLANT) = CONC. IN TISSUE (DRY WT.)/CONC. IN SOI
     $L  (UNITLESS) = ',1PE10.3)
      WRITE(IWB,240)
  240 FORMAT(/,24X,'BCFAN (ANIMAL) = CONC. IN TISSUE (FRESH WT.)/CONC. I
     $N DIET  (UNITLESS):')
      LOGKOW=ALOG10(KOW)
      IF(LOGKOW.GE.3.5)GO TO 260
      WRITE(IWB,250)
  250 FORMAT(41X,'* BCFAN OF THE COMPOUND IS LIKELY TO BE LESS THAN 0.1'
     $,////)
      GO TO 272
  260 WRITE(IWB,270)
  270 FORMAT(41X,'* THE COMPOUND MAY BE BIOACCUMULATED WITH A BCFAN OF A
     $T LEAST 0.1',////)
  272 CONTINUE
C
C     THE FOLLOWING PARAMETERS ARE CONSTANTS USED IN THE EQUATIONS BELOW
C
      TELAM=TE*LAMBDA
      BCFPRS=BCFPL/RS
      PLFAC=(R/(YV*LAMBDA))*(1.0-((1.0-EXP(-TELAM))/TELAM))/30.0
  273 WRITE(IWB,274)
  274 FORMAT('0',26X,'* CONCENTRATIONS IN AQUATIC ORGANISMS AND TERRESTR
     $IAL PLANTS (FORAGE) IN UG/G',/)
      WRITE(IWB,276)
  276 FORMAT(25X,'LAKE',23X,'RIVER',21X,'ESTUARY',15X,'OCEAN',5X,'SOIL-A
     $IR OPTION')
      WRITE(IWB,278)
  278 FORMAT(16X,3(2X,'AQUATIC',5X,'PLANTS',7X),2X,'AQUATIC',8X,'PLANTS'
     $,/)
      GO TO 290
  280 IF(COVFLG.EQ.YES)RETURN
  290 CONTINUE
      IF(WATBOD.EQ.NO)GO TO 600
C
C
      IF(LAKE.NE.YES)GO TO 300
C
C     COMPUTE CONCENTRATIONS IN AQUATIC ORGANISMS & TERRESTRIAL PLANTS
C     FOR LAKE SIMULATION.
C
      CONAQL=BCFAQ*(CONL1+CONL2+CONL3)/1.0E+6
      IF(AREASL.EQ.0.0)GO TO 300
      CONPLL=BCFPRS*SCONUL+PLFAC*ASDEPL/AREASL
C
C
  300 IF(RIVER.NE.YES)GO TO 400
C
C     COMPUTE CONCENTRATIONS IN AQUATIC ORGANISMS & TERRESTRIAL PLANTS
C     FOR RIVER SIMULATION. (USE MAXIMUM CONCENTRATION IN RIVER)
C
      CONRIV=0.0
      DO 350 I=1,NR
  350 CONRIV=AMAX1(CONRIV,(CONR1(I)+CONR2(I)+CONR3(I)))
      CONAQR=BCFAQ*CONRIV/1.0E+6
      IF(AREASR.EQ.0.0)GO TO 400
      CONPLR=BCFPRS*SCONUR+PLFAC*ASDEPR/AREASR
C
C
  400 IF(ESTU.NE.YES)GO TO 500
C
C     COMPUTE CONCENTRATIONS IN AQUATIC ORGANISMS & TERRESTRIAL PLANTS
C     FOR ESTUARY SIMULATION (USE MAXIMUM CONCENTRATION IN ESTUARY).
C
      CONEST=0.0
      NPTSP1=NPTSE+1
      DO 450 I=1,NPTSP1
  450 CONEST=AMAX1(CONEST,(CNCED1(I)+CNCED2(I)+CNCED3(I)),
     &         (CNCEU1(I)+CNCEU2(I)+CNCEU3(I)))
      CONAQE=BCFAQ*CONEST/1.0E+6
      IF(AREASE.EQ.0.0)GO TO 500
      CONPLE=BCFPRS*SCONUE+PLFAC*ASDEPE/AREASE
C
C
  500 IF(OCEAN.NE.YES)GO TO 700
C
C     COMPUTE CONCENTRATIONS IN AQUATIC ORGANISMS FOR OCEAN (USE MAXIMUM
C     CONCENTRATION IN OCEAN)
C
      CONOCN=0.0
      DO 550 I=1,NPTSO
  550 CONOCN=AMAX1(CONOCN,(CONO1(I)+CONO2(I)+CONO3(I)))
      CONAQO=BCFAQ*CONOCN/1.0E+6
      GO TO 700
C
C
C     HERE, SIMULATION CONSIDERS ONLY AIR-SOIL INTERACTIONS; IE NO
C     WATER BODY IS CONSIDERED.
C
  600 CONPLS=BCFPRS*SCONUS+PLFAC*ASDEPS/AREAS
C
C     WRITE OUT RESULTS
C
  700 WRITE(IWB,800)AMO(IMO),CONAQL,CONPLL,CONAQR,CONPLR,CONAQE,CONPLE,
     $                CONAQO,CONPLS
  800 FORMAT(10X,A4,2X,3(1PE10.3,2X,1PE10.3,5X),1PE10.3,5X,1PE10.3)
      IF(IMO.EQ.12.AND.IYR.EQ.JYRS)GO TO 900
      RETURN
  900 WRITE(IWB,1000)
 1000 FORMAT(////,56X,'* CAUTION',/)
      WRITE(IWB,1100)
 1100 FORMAT(27X,'NO CONFIDENCE SHOULD BE PLACED IN THE METHODS USED TO
     $ CALCULATE')
      WRITE(IWB,1200)
 1200 FORMAT(27X,'CONCENTRATION IN AQUATIC ORGANISMS OR IN TERRESTRIAL P
     $LANTS VIA ROOT')
      WRITE(IWB,1300)
 1300 FORMAT(27X,'UPTAKE, OR TO EVALUATE BIOACCUMULATION POTENTIAL IN TE
     $RRESTRIAL ANIMALS, IF:',/)
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      WRITE(IWB,1400)
1400  FORMAT(31X,'1) THE COMPOUND IS A COVALENTLY BONDING COMPOUND,')
      WRITE(IWB,1500)
1500  FORMAT(31X,'2) THE COMPOUND IS APPRECIABLY DEGRADED IN THE BIOTIC
     $PHASE,')
      WRITE(IWB,1600)
1600  FORMAT(31X,'3) THE DOMINANT CONCENTRATING PHASE IN THE ORGANISM IS
     $ NOT A LIPID,')
      WRITE(IWB,1700)
1700  FORMAT(31X,'4) THE KOW EQUALS OR EXCEEDS 1.0E+6, OR IF')
      WRITE(IWB,1800)
1800  FORMAT(31X,'5) THE CALCULATED BCF VALUE IS BELOW 10.',/)
      WRITE(IWB,1900)
1900  FORMAT(27X,'IT SHOULD FURTHER BE RECOGNIZED THAT THE METHOD IS NOT
     $ ABSOLUTE')
      WRITE(IWB,2000)
2000  FORMAT(27X,'BECAUSE STERIC PROPERTIES AND SIZE OF THE CHEMICAL COM
     $POUND, IN ADDITION')
      WRITE(IWB,2100)
2100  FORMAT(27X,'TO LIPOPHILICITY, AFFECT THE PREDICTED ACCUMULATION IN
     $ TISSUES.')
      WRITE(IWB,2200)
2200  FORMAT(27X,'ALSO, A POSSIBLY SIGNIFICANT DEGREE OF UNCERTAINTY SHO
     $ULD')
      WRITE(IWB,2300)
2300  FORMAT(27X,'BE ATTACHED TO ESTIMATED CONCENTRATIONS FOR ANY ONE OR
     $GANISM')
      WRITE(IWB,2400)
2400  FORMAT(27X,'DUE TO DIFFERENCES IN FRACTIONAL LIPID COMPOSITION.')
      RETURN
      END
      REAL FUNCTION CAVGE(X)
      COMMON/AIRPAR/QS(12,10),UW(12,10),HMIX(12,10),CTYLTH,
     $              UDG,UDP,WRATG,WRATP,AK,HS,VS,SRAD,RHO,ENTPY
      COMMON/CAVPAR/HEFFIV,XMAX,HMIXZ,U,VG,UDPW,DEPFAC
      PI=3.1415927
      SIGZMX=2.0*(HMIXZ-HEFFIV)/2.15
C
C CALCULATE SIGMA SUB Y AND Z
C
      SIGMAY=0.08*X/SQRT(1.0+0.0001*X)
      SIGMAZ=0.06*X/SQRT(1.0+0.0015*X)
      IF(SIGMAZ.GT.SIGZMX) SIGMAZ=SIGZMX
C
C INTEGRATE CAVGE FROM A TO X-FINAL BY D01AJF TO FIND AVERAGE AIR CONCENTRATION
C
      CAVGE=EXP(-0.5*((HEFFIV-VG*X/U)/SIGMAZ)**2-SQRT(2.0/PI)*UDPW/U
     $*DEPFAC-AK*X/U)/(2.0*SQRT(2.0*PI)*SIGMAY*SIGMAZ*U)
C
      RETURN
      END
      REAL FUNCTION DEPAVG(X)
      COMMON/AIRPAR/QS(12,10),UW(12,10),HMIX(12,10),CTYLTH,
     $             UDG,UDP,WRATG,WRATP,AK,HS,VS,SRAD,RHO,ENTPY
      COMMON/CAVPAR/HEFFIV,XMAX,HMIXZ,U,VG,UDPW,DEPFAC
      SIGZMX=2.0*(HMIXZ-HEFFIV)/2.15
      SIGMAZ=0.06*X/SQRT(1.0+0.0015*X)
C
C CALCULATE SIGMA SUB Z
C
      IF(SIGMAZ.GT.SIGZMX)SIGMAZ=SIGZMX
C
C CALCULATE AVERAGE DEPLETION - THIS IS INTEGRATED FROM A TO X-FINAL
C BY ROUTINE D01AJF
C
      DEPAVG=EXP(-0.5*((HEFFIV-VG*X/U)/SIGMAZ)**2)/SIGMAZ
C
      RETURN
      END
      SUBROUTINE FUNLAU(DIASED,DENSED,DENWAT,WDEPTH,SLOPE,TCRIT,
     $                     FUNC,TOPFAC,RATIO)
      DIMENSION SVFL(26),F(26),BFUNC(26),CFUNC(26),DFUNC(26),DIAVFL(12),
     $ VFL(12),BVFALL(12),CVFALL(12),DVFALL(12),DIATHE(22),SHIELD(22),
     $ BTHETA(22),CTHETA(22),DTHETA(22)
C
C DIATHE, SHIELD, BTHETA, CTHETA, & DTHETA ARE PARAMETERS
C NEEDED IN SPLINE CALCULATION OF SHIELDS FACTOR (THETA) BELOW.
C
      DATA DIATHE/.01,.015,.02,.03,.04,.06,.08,.1,.15,.2,.3,.4,.6,.8,
     $ 1.0,1.5,2.0,3.0,4.0,6.0,8.0,10.0/
      DATA SHIELD/1.0,.60,.43,.275,.20,.17,.12,.085,.06,.05,.038,.034,
     $ .032,.033,.034,.04,.045,.053,.056,.059,.06,.06/
      DATA BTHETA/-112.5423,-51.66603,-22.79358,-10.40648,-4.580516,
     $ -1.203952,-2.603676,-1.131346,-.1963915,-.1830883,
     $ -.06868714,-.02216312,.0003529924,.005751148,.006642417,
     $ .01262521,.008856734,.005609170,.001706586,.001042143,
     $ .0001248412,-.00004150783/
      DATA CTHETA/7350.127,4825.127,949.3631,289.3469,293.2492,
     $ -124.421,54.43484,19.18166,-.4825736,.7486376,.3953741,
     $ .06986621,.04271434,-.01572356,.02017991,-.008214317,
     $ .0006773615,-.003924926,.00002234224,-.0003545637,
     $-.0001040873,.00002091275/
      DATA DTHETA/-168333.3,-258384.3,-22000.54,130.0753,-6961.17,
     $ 2980.931,-587.553,-151.0949,8.208074,-1.177545,
     $ -1.085026,-.04525312,-.0973965,.05983912,-.01892948,
     $ .005927786,-.001534016,.001315756,-.00006281766,
     $ .00004174608,.00002083333,.00002083333/
C
C DIAVFL, VFL, BVFALL, CVFALL, DVFALL ARE PARAMETERS NEEDED IN SPLINE
C CALCULATION OF FALL VELOCITY (VFALL) BELOW.
C
      DATA DIAVFL/.035,.05,.08,.1,.2,.5,.8,1.,2.,5.,8.,10./
      DATA VFL/.001,.0021,.0053,.0084,.028,.062,.082,.094,.130,
     $ .20,.245,.270/
      DATA BVFALL/.06516542,.0822833,.1359694,.1702466,.1901943,
     $ .07170594,.06298195,.05558953,.02601584,.01910471,
     $ .01256532,.01287912/
      DATA CVFALL/.4923909,.6488011,1.140735,.5731256,-.3736484,
     $ -.02131277,-.00776711,-.0291949,-.0003787943,-.001924914,
     $ -.0002540026,.0004111841/
      DATA DVFALL/3.475783,1.465927,-9.460148,-3.155913,.3914841,
     $ .01505064,-.03571206,.00960537,-.0001717911,.0001855591,
     $ .0001111111,.000111111/
C
C SVFL, F, BFUNC, CFUNC, DFUC ARE PARAMETERS NEEDED IN SPLINE CALCULATION
C OF LAURSEN'S FUNCTION (FUN) BELOW.
C
      DATA SVFL/-4.60517,-3.91202,-3.21887,-2.81341,-2.52573,-2.30259,
     $ -1.60944,-.91629,-.5108,-.22314,0.,.69315,1.38629,1.79176,
     $ 2.07944,2.30259,2.9957,3.68888,4.09434,4.38203,4.60517,5.29832,
     $ 5.99146,6.39693,6.6846,6.90776/
      DATA F/1.253,1.611,1.50,1.666,1.750,1.792,1.900,2.197,2.300,
     $ 3.503,3.773,3.996,4.87,5.700,6.397,6.867,8.033,9.243,9.900,
     $ 10.127,10.375,10.545,1.682,10.799,10.878,10.933/
      DATA BFUNC/.3200040,.300600,.3100260,.3101113,.2200750,.1600300,
     $ .2907453,.4489659,.4939646,.7892218,.9613132,1.469371,2.224274,
     $ 2.227120,2.096494,2.233934,1.642620,1.487729,1.199183,.6293903,
     $ .6281968,.2352389,.2356600,.2792161,.2636840,.2254239/
      DATA CFUNC/-.007068473,.01006856,-.03320577,.2827604,-.5995552,
     $ .2229258,-.006787031,.2350501,-.1240681,1.150371,-.3791451,
     $ 1.112114,-.02300823,.03002671,-.4840906,1.100025,-1.953107,
     $ 1.729647,-2.441297,.4607183,-.466067,-.1008493,.1014569,
     $ .005964327,-.05995511,-.1114997/
      DATA DFUNC/.008241137,-.02081047,.2597594,-1.022335,1.228592,
     $ -.1104696,.1162986,-.2952353,1.476635,-2.284838,.7171412,
     $ -.5458842,.04359956,-.5957051,2.366401,-1.46824,1.771023,
     $ -3.428981,3.362434,-1.384460,.1756319,.09728969,-.07850358,
     $ -.07638051,-.0769955,-.0769955/
      IWP=13
C
C DIASED IS SEDIMENT MEDIAN DIAMETER IN MM.
C
      DIA=DIASED
      IF(DIASED.GE.DIATHE(1).AND.DIASED.LE.DIATHE(22))GO TO 10
      IF(DIASED.LT.DIATHE(1))DIA=DIATHE(1)
      IF(DIASED.GT.DIATHE(22))DIA=DIATHE(22)
      WRITE(IWP,5)
 5    FORMAT(1X,'WARNING IN FUNLAU: THE SEDIMENT DIAMETER IS OUTSIDE THE
     $ BOUNDS OF THE SHIELDS FACTOR CURVE; CODE USED ENDPOINT')
 10   THETA=SPLEVA(22,DIA,DIATHE,SHIELD,BTHETA,CTHETA,DTHETA)
C
C DIASDM IS SEDIMENT MEDIAN DIAMETER IN M.
C
      DIASDM=0.001*DIASED
C
C CONVERT DENSITY OF SEDIMENT (DENSED) AND DENSITY OF WATER
C (DENWAT) FROM G/CM**3 TO KG/M**3.
C
      DENSED=DENSED*1000.0
      DENWAT=DENWAT*1000.0
C
C CALCULATE CRITICAL TRACTIVE FORCE FOR BEGINNING OF
C SEDIMENT TRANSPORT.
C
      TCRIT=THETA*(DENSED-DENWAT)*DIASDM
      DIADTH=DIASDM/WDEPTH
C
C COMPUTE FACTOR (TOPFAC) USED IN BOUNDARY SHEAR EQUATION IN SEDCON.
C
      TOPFAC=DENWAT*(DIADTH)**(1./3.)/590.0928
C
C CALCULATE RATIO OF SEDIMENT DIAMETER TO WATER DEPTH RAISED
C TO THE 7/6 POWER (TO BE USED IN LAURSEN'S FORMULA BELOW).
C
      RATIO=DIADTH**(7.0/6.0)
C
C CALCULATE SQ. ROOT OF BOUNDARY SHEAR (SHEAR) USED IN LAURSEN'S
C FORMULA BELOW.
C
      SHEAR=SQRT(WDEPTH*SLOPE*9.80665)
C
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C COMPUTE FALL VELOCITY (M/S).
C
      DIA=DIASED
      IF(DIASED.GE.DIAVFL(1).AND.DIASED.LE.DIAVFL(12))GO TO 20
      IF(DIASED.LT.DIAVFL(1))DIA=DIAVFL(1)
      IF(DIASED.GT.DIAVFL(12))DIA=DIAVFL(12)
      WRITE(IWP,15)
 15   FORMAT(1X,'WARNING IN FUNLAU: THE SEDIMENT DIAMETER IS OUTSIDE THE
     $ BOUNDS OF THE FALL VELOCITY CURVE; CODE USED ENDPOINT')
 20   VFALL=SPLEVA(12,DIA,DIAVFL,VFL,BVFALL,CVFALL,DVFALL)
C
C CALCULATE FUNCTION NEEDED IN LAURSEN'S FORMULA. LOG'S USED FOR ACCURACY.
C
      SHEVFL=ALOG(SHEAR/VFALL)
      IF(SHEVFL.GE.SVFL(1).AND.SHEVFL.LE.SVFL(26))GO TO 50
      IF(SHEVFL.LT.SVFL(1))SHEVFL=SVFL(1)
      IF(SHEVFL.GT.SVFL(26))SHEVFL=SVFL(26)
      WRITE(IWP,25)
 25   FORMAT(1X,'WARNING IN FUNLAU: THE BOTTOM SHEAR VELOCITY DIVIDED BY
     $ THE FALL VELOCITY IN LAURSENS FUNCTION IS OUTSIDE THE BOUNDS OF L
     $AURSENS CURVE; CODE USED ENDPOINT')
 50   FUNC=SPLEVA(26,SHEVFL,SVFL,F,BFUNC,CFUNC,DFUNC)
      FUNC=EXP(FUNC)
      RETURN
      END
      SUBROUTINE OUTPUT(MON,IYR)
      COMMON/OUT/ACMAXL,AVAIRL,AVAIRR,AVAIRE,AWDEPL,AWDEPR,AWDEPE,
     $           ASDEPL,ASDEPR,ASDEPE,WVOLAL,WVOLAR,WVOLAE,SVOLAL,
     $           SVOLAR,SVOLAE,SWSURL,SWSURR,SWSURE,SWGRWL,SWGRWR,
     $           SWGRWE,SCONUL,SCONUR,SCONUE,SCONLL,SCONLR,SCONLE,
     $           CONL1,CONL2,CONL3,CONR1(20),CONR2(20),CONR3(20),
     $           CNCED1(11),CNCED2(11),CNCED3(11),CNCEU1(11),CNCEU2(11),
     $           CNCEU3(11),XESTY(11),CONO1(10),CONO2(10),CONO3(10),
     $           RESUSE,WASHL,WASHR,WASHE,ACMAXR,ACMAXE,ACMAXS,
     $           AVAIRS,ASDEPS,SVOLAS,SWGRWS,SCONUS,SCONLS,RESUSS,
     $           RESUSL,RESUSR,SCONML,SCONMR,SCONME,SCONMS,SWSURS,
     $           WASHS,AREA1(3)
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $            ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/WPARL/WVELL(12,10),WMINL(12,10),WMTLKE,AREALK,
     $            WDEPL,WVOLL
      COMMON/WPARR/WVELR(12,10),WMINR(12,10),WMTRIV(20),
     $            NR,WWIDR,WLENR,WDEPR,WVOLR,WMTOLD,AREAR
      COMMON/WPARE/WVELE(12,10),WMINE(12,10),TIDMAX,EL,WWIDE,
     $            WLENE,WDEPE,NPTSE,AREAE
      COMMON/WPARO/WVELO(12,10),WCINO(12,10),BO,XOCEAN,NPTSO
      REAL LAKE,NO
      DIMENSION AMO(12)
      DATA YES/4H YES/,AREA/4HAREA/,NO/4H  NO/
      DATA AMO/' OCT',' NOV',' DEC',' JAN',' FEB',' MAR',
     $' APR',' MAY',' JUN',' JUL',' AUG',' SEP'/
C
C LAKE RESULTS ARE WRITTEN WITH UNIT # IWL, RIVER RESULTS WITH UNIT
C # IWR, ESTUARY RESULTS WITH UNIT # IWE, & OCEAN RESULTS WITH UNIT
C # IWO. IF NO WATER BODY IS CONSIDERED, UNIT # IWL IS USED TO WRITE
C THE RESULTS.
C
      IWL=14
      IWR=15
      IWE=16
      IWO=17
      IF(MON.GT.1)GO TO 100
      IF(WATBOD.EQ.NO)GO TO 96
C
C
      IF(LAKE.NE.YES)GO TO 30
      WRITE(IWL,10)
 10   FORMAT('1',33X,'MONTHLY POLLUTANT CONCENTRATIONS AND INTERACTION T
     $ERMS')
      WRITE(IWL,20)
 20   FORMAT('0',50X,'WATER BODY IS A LAKE')
      WRITE(IWL,22)AREALK
 22   FORMAT('0',33X,'CONTAMINATED WATER (SURFACE AREA) IN M**2  = ',
     $1PE10.3)
      WRITE(IWL,24)AREA1(1)
 24   FORMAT(34X,'CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 = ',
     $1PE10.3)
      WRITE(IWL,25)IYR
 25   FORMAT('0',56X,'YEAR ',I2)
C
C
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 30   IF(RIVER.NE.YES)GO TO 50
      WRITE(IWR,10)
      WRITE(IWR,40)
 40   FORMAT('0',50X,'WATER BODY IS A RIVER')
      WRITE(IWR,45)
 45   FORMAT(1X,50X,'IR IS THE REACH NUMBER')
      WRITE(IWR,22)AREAR
      WRITE(IWR,24)AREA1(2)
      WRITE(IWR,25)IYR
C
C
 50   IF(ESTU.NE.YES)GO TO 70
      WRITE(IWE,10)
      WRITE(IWE,60)
 60   FORMAT('0',48X,'WATER BODY IS AN ESTUARY')
      WRITE(IWE,65)
 65   FORMAT(1X,24X,'X IS DISTANCE FROM SOURCE IN METERS; + FOR DOWNSTRE
     $AM AND - FOR UPSTREAM')
      WRITE(IWE,22)AREAE
      WRITE(IWE,24)AREA1(3)
      WRITE(IWE,25)IYR
C
C
 70   IF(OCEAN.NE.YES)GO TO 100
      WRITE(IWO,80)
 80   FORMAT('1',28X,'MONTHLY POLLUTANT CONCENTRATIONS')
      WRITE(IWO,90)
 90   FORMAT('0',33X,'WATER BODY IS AN OCEAN')
      WRITE(IWO,92)
 92   FORMAT(27X,'X IS DISTANCE FROM SOURCE IN METERS')
      WRITE(IWO,95)IYR
 95   FORMAT('0',40X,'YEAR ',I2)
      WRITE(IWO,103)
 103  FORMAT(33X,'CONCENTRATIONS (UG/M**3)')
      WRITE(IWO,104)
 104  FORMAT(//,19X,'WATER (NEUTRAL)',
     $3X,'WATER (IONIC)',3X,'WATER (ADSORBED)')
      GO TO 100
C
C
 96   WRITE(IWL,10)
      WRITE(IWL,97)
 97   FORMAT('0',46X,'NO WATER BODY IS CONSIDERED')
      WRITE(IWL,24)AREA1(1)
      WRITE(IWL,25)IYR
      GO TO 500
 100  CONTINUE
      IF(WATBOD.EQ.NO)GO TO 500
C
C
      IF(LAKE.NE.YES)GO TO 200
      WRITE(IWL,105)AMO(MON)
 105  FORMAT(1X,3X,A4)
      WRITE(IWL,110)
 110  FORMAT(1X,'  CONCS ',3X,'MAXIMUM AIR',3X,'AVERAGE AIR',5X,
     $'WAT NEUTRAL',1X,' WAT IONIC ',2X,'WAT ADSORBED',2X,
     $'UPPER SOIL',2X,'MIDDLE SOIL',2X,'LOWER SOIL',2X,'RESUSPENSION')
      ACMAXL=ACMAXL+RESUSL
      AVAIRL=AVAIRL+RESUSL
      IF(AIRFLG.EQ.AREA)GO TO 130
      WRITE(IWL,120)ACMAXL,AVAIRL,CONL1,CONL2,CONL3,SCONUL,SCONML,
     $               SCONLL,RESUSL
 120  FORMAT(1X,'(UG/M**3)  ',2(1PE10.3,4X),2X,1PE10.3,
     $2X,6(1PE10.3,3X))
      GO TO 150
 130  WRITE(IWL,140)AVAIRL,CONL1,CONL2,CONL3,SCONUL,SCONML,SCONLL,RESUSL
 140  FORMAT(1X,'(UG/M**3)  ***********',3X,1PE10.3,6X,1PE10.3,
     $2X,6(1PE10.3,3X))
 150  WRITE(IWL,160)
 160  FORMAT(1X,'  RATES   ','DEP ON WATER',3X,'DEP ON SOIL',5X,
     $'VOLAT WATER ',1X,'VOLAT SOIL ',1X,'SURF RUNOFF'
     $,2X,'GRWTR RUNOFF',2X,'WASHLOAD')
      WRITE(IWL,170)AWDEPL,ASDEPL,WVOLAL,SVOLAL,SWSURL,
     $               SWGRWL,WASHL
 170  FORMAT(1X,'(UG/MON)   ',2(1PE10.3,4X),2X,1PE10.3,2X,
     $4(1PE10.3,3X),/)
C
C
 200  IF(RIVER.NE.YES)GO TO 300
      WRITE(IWR,105)AMO(MON)
      WRITE(IWR,110)
      IR=1
      ACMAXR=ACMAXR+RESUSR
      AVAIRR=AVAIRR+RESUSR
      IF(AIRFLG.EQ.AREA)GO TO 215
      WRITE(IWR,210)ACMAXR,AVAIRR,IR,CONR1(1),CONR2(1),CONR3(1),
     $               SCONUR,SCONMR,SCONLR,RESUSR
 210  FORMAT(1X,'(UG/M**3) ',1X,1PE10.3,4X,1PE10.3,' IR=',I2,1PE10.3,
     $2X,6(1PE10.3,3X))
      GO TO 218
 215  WRITE(IWR,217)AVAIRR,IR,CONR1(1),CONR2(1),CONR3(1),
     $               SCONUR,SCONMR,SCONLR,RESUSR
 217  FORMAT(1X,'(UG/M**3)  ***********',3X,1PE10.3,' IR=',I2,
     $1PE10.3,2X,6(1PE10.3,3X))
 218  IF(NR.EQ.1)GO TO 235
      DO 220 IR=2,NR
 220  WRITE(IWR,230)IR,CONR1(IR),CONR2(IR),CONR3(IR)
 230  FORMAT(1X,36X,'IR=',I2,1PE10.3,2X,2(1PE10.3,3X))
 235  CONTINUE
      WRITE(IWR,160)
      WRITE(IWR,170)AWDEPR,ASDEPR,WVOLAR,SVOLAR,SWSURR,
     $               SWGRWR,WASHR
C
C
 300  IF(ESTU.NE.YES)GO TO 400
      WRITE(IWE,105)AMO(MON)
      WRITE(IWE,110)
      ISEGT=ESGTV(1)
      ACMAXE=ACMAXE+RESUSE
      AVAIRE=AVAIRE+RESUSE
      IF(AIRFLG.EQ.AREA)GO TO 320
      WRITE(IWE,310)ACMAXE,AVAIRE,ISEGT,CNCES1(1),CNCES2(1),CNCES3(1),
     $                  SCONUE,SCONME,SCONLE,RESUSE
 310  FORMAT(1X,'(UG/M**3) ',1X,1PE10.3,4X,1PE9.2,' X=',I6,1PE10.3,
     $6(1PE10.3,3X))
      GO TO 340
 320  WRITE(IWE,330)AVAIRE,IXEST,CNCEU1(1),CNCEU2(1),CNCEU3(1),
     $                  SCONUE,SCONME,SCONLE,RESUSE
 330  FORMAT(1X,'(UG/M**3)  ***********',3X,1PE9.2,' X=',I6,
     $1PE10.3,6(1PE10.3,3X))
 340  DO 350 I=1,NPTSE
      IE=I+1
      IXEST=XESTY(IE)
      WRITE(IWE,360)IXEST,CNCED1(IE),CNCED2(IE),CNCED3(IE)
      IXEST=-IXEST
 350  WRITE(IWE,360)IXEST,CNCEU1(IE),CNCEU2(IE),CNCEU3(IE)
 360  FORMAT(1X,35X,'X=',I6,1PE10.3,2(1PE10.3,3X))
      WRITE(IWE,160)
      WRITE(IWE,170)AWDEPE,ASDEPE,WVOLAE,SVOLAE,SWSURE,
     $                  SWGRWE,WASHE
C
C
 400  IF(OCEAN.NE.YES)RETURN
      WRITE(IWO,405)AMO(MON)
 405  FORMAT(2X,A4)
      OCNPT=0.
      DO 420 I=1,NPTSO
      OCNPT=OCNPT+XOCEAN
 420  WRITE(IWO,410)OCNPT,CONO1(I),CONO2(I),CONO3(I)
 410  FORMAT(7X,'X= ',E9.2,2X,3(1PE10.3,7X))
      RETURN
C
C
 500  CONTINUE
      WRITE(IWL,105)AMO(MON)
      WRITE(IWL,110)
      ACMAXS=ACMAXS+RESUSS
      AVAIRS=AVAIRS+RESUSS
      IF(AIRFLG.EQ.AREA)GO TO 520
      WRITE(IWL,510)ACMAXS,AVAIRS,SCONUS,SCONMS,SCONLS,RESUSS
 510  FORMAT(1X,'(UG/M**3)  ',2(1PE10.3,4X),2(2X,' *********'),3X,
     $' *********',3X,4(1PE10.3,3X))
      GO TO 540
 520  WRITE(IWL,530)AVAIRS,SCONUS,SCONMS,SCONLS,RESUSS
 530  FORMAT(1X,'(UG/M**3)  ***********',3X,1PE10.3,6X,' *********',
     $2X,' *********',3X,' *********',3X,4(1PE10.3,3X))
 540  WRITE(IWL,160)
      WRITE(IWL,550)ASDEPS,SVOLAS,SWSURS,SWGRWS,WASHS
 550  FORMAT(1X,'(UG/MON)   ***********',3X,1PE10.3,6X,' *********',
     $3X,4(1PE10.3,3X),/)
      RETURN
      END
 SUBROUTINE READIN
 COMMON/MEDIA/AWMINR,AWIOUR,WAMOUR(20),AWMINL,AWMOUL,
$               WAMOUL,SWIINL,SWMINR,AWMINE,AWMOUE,SWMINE,WAMOUE,
$               SAMOUL,ASIIDL,ASMIWL,SAMOUR,ASMIDR,ASMIWR,SAMOUE,
$               ASMIDE,ASIIWE,ASMOWL,ASMODL,ASMODR,ASMOWR,
$               ASMODE,ASIOWE,SWMOUL,SWMOUR,SWMOUE,CUMLKE,
$               CLMLKE,CUIRIV,CLMRIV,CUMEST,CLMEST,ASMODS,ASMOWS,
$               ASMIDS,ASIIWS,SAMOUS,CUMS,CLMS,SUMLKE,SLMLKE,CUSALK,
$               CLSALK,LI(CUL,LIGCLL,SUMRIV,SLMRIV,CUSARV,CLSARV,
$               LIGCUR,LI(CLR,SUMEST,SLMEST,CUSAES,CLSAES,LIGCUE,
$               LIGCLE,SUIS,SLMS,CUSAS,CLSAS,LIGCUS,LIGCLS,CMMLKE,
$               CMMRIV,CMIEST,CMMS,SMMLKE,SMMRIV,SMMEST,SMMS,
$               CMSALK,CM:ARV,CMSAES,CMSAS,LIGCML,LIGCMR,LIGCME,
$               LIGCMS
 COMMON/FLAGS/AIRFLG,AIIPOL,TRICON,LAKE,RIVER,
$               ESTU,OCEAI,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
 COMMON/ALPHAS/A1L,A2L,/3L,A1R,A2R,A3R,A1E,A2E,A3E,
$                A1O,A2O,/3O
 COMMON/AIRPAR/QS(12,10),UW(12,10),HMIX(12,10),CTYLTH,
$                UDG,UDP,WRATG,WRATP,AK,HS,VS,SRAD,RHO,ENTPY
 COMMON/WPARL/WVELL(12,0),WMINL(12,10),WMTLKE,AREALK,
$               WDEPL,WVOL
 COMMON/WPARR/WVELR(12,0),WMINR(12,10),WMTRIV(20),
$               NR,WWIDR,LENR,WDEPR,WVOLR,WMTOLD,AREAR
 COMMON/WPARE/WVELE(12,0),WMINE(12,10),TIDMAX,EL,WWIDE,
$               WLENE,WDEE,NPTSE,AREAE
 COMMON/CAVPAR/HEFFIV,XRAX,HMIXZ,U,VG,UDPW,DEPFAC
 COMMON/SPARS/ARS,AREAS(LENS
 COMMON/SPARL/ARL,AREASL,XSOIL
 COMMON/SPARR/ARR,AREAS
 COMMON/SPARE/ARE,AREAS
 COMMON /AP/ GEOM(20),LAD(6),RUNLO(6),RUNM1(10,12),RUNM2(10,12)
 COMMON /HB/ HYDBAL(13,9)
 COMMON/SDPARE/SEDCE(12)0),CONSDE
 COMMON/SDPARO/SEDCO(12)0),CONSDO
 COMMON/SDPARR/SEDCR(12)0),DIASDR,DENSDR,DENWR,SLOPER,CONSDR
 COMMON/SDPARL/SEDCL(12)0),DIASDT,DENSDT,DENWT,SLOPET,WDEPT,CONSDL
 COMMON/EQUIL/DISK,HPLUL,HPLUSR,HPLUSE,HPLUSO,
$                      SWKSL,SWKSWR,SWKSWE,SWKSWO
 COMMON/WPARO/WVELO(12,1),WCINO(12,10),SO,XOCEAN,NPTSO
 COMMON/WRATES/WKVL,WKP(WKOL,WKBL,WKHL,
$                WKVR,WKP(WKOR,WKBR,WKHR,
$                WKVE,WKP(WKOE,WKBE,WKHE,
$                WKVO,WKP(WKOO,WKBO,WKHO
 COMMON /EX/ JOUN,LEVEL(EE,JSO,JCH,JNUT,JAPPL,JYRS
 COMMON /TI/ TITLES(5,1)
 DIMENSION AMO(12)
 REAL LAKE,NO,NONE
 DATA AMO/' OCT',' NOV', DEC',' JAN',' FEB',' MAR',
$' APR',' MAY',' JUN','UL',' AUG',' (EP'/
 DATA YES/4H YES/,NO/4H NO/,NONE/4HNONE/,AREA/4HAREA/,
$      POINT/4HPOIN/,PA/4HPART/,GAS/4H GAS/,ACID/4HACID/,
$      BASE/4HBASE/
C
C INP UNIT 5 FOR FILE READING MODEL FLAGS
C
```

```
      IRF=10
C
C IRA UNIT # FOR FILE READING IN AIR PARAMETERS
C
      IRA=11
C
C IRW UNIT # FOR FILE READING IN WATER PARAMETERS
C
      IRW=12
C
C IWP UNIT # FOR OUTPUT MESSAGES (ALSO, OUTPUTS INPUT DATA)
C
      IWP=13
C
C IWG UNIT # FOR GENERAL OUTPUT FILE
C
      IWG=13
C
      READ(IRF,10) AIRFLG,AIRPOL
   10 FORMAT(A4,6X,A4,6X,A4)
      READ(IRF,10) LAKE,SEDLKE,TRICON
      READ(IRF,10) RIVER,SEDRIV
      READ(IRF,10) ESTU,DISFLG
      READ(IRF,10) OCEAN
      WATBOD=YES
      IF(LAKE.EQ.NO.AND.RIVER.EQ.NO.AND.ESTU.EQ.NO.AND.OCEAN.EQ.NO)
     $   WATBOD=NO
      IF(WATBOD.NE.NO)READ(IRF,10)CHMFLG
      WRITE(IWP,1)
 1    FORMAT('1',44X,'MODEL FLAGS THAT DETERMINE WHAT USER INPUTS')
      WRITE(IWP,2)
 2    FORMAT('0',26X,'OPTION CHOSEN',6X,'NAME',21X,'MEANING',/)
      IF(AIRFLG.EQ.POINT)WRITE(IWP,3)
 3    FORMAT(35X,'POINT',5X,'AIRFLG',5X,'SIGNIFIES AIR POINT SOURCE')
      IF(AIRFLG.EQ.AREA)WRITE(IWP,4)
 4    FORMAT(36X,'AREA',5X,'AIRFLG',5X,'SIGNIFIES AIR AREA SOURCE')
      IF(AIRFLG.EQ.NONE)WRITE(IWP,5)
 5    FORMAT(36X,'NONE',5X,'AIRFLG',5X,'SIGNIFIES NO AIR SOURCE')
      IF(AIRPOL.EQ.GAS)WRITE(IWP,6)
 6    FORMAT(37X,'GAS',5X,'AIRPOL',5X,'SIGNIFIES POLLUTANT IS A GAS')
      IF(AIRPOL.EQ.PART)WRITE(IWP,7)
 7    FORMAT(27X,'(PART)ICULATE',5X,'AIRPOL',5X,'SIGNIFIES POLLUTANT IS
     $A PARTICULATE')
C
C
      IF(LAKE.EQ.YES)WRITE(IWP,8)
 8    FORMAT(37X,'YES',6X,'LAKE',6X,'SIGNIFIES THAT A LAKE IS BEING CONS
     $IDERED')
      IF(LAKE.EQ.NO)WRITE(IWP,9)
 9    FORMAT(38X,'NO',6X,'LAKE',6X,'SIGNIFIES THAT A LAKE IS NOT BEING C
     $ONSIDERED')
      IF(LAKE.EQ.NO)GO TO 21
      IF(LAKE.EQ.YES)GO TO 1020
      WRITE(IWP,1010)LAKE
 1010 FORMAT(1X,'ERROR IN DATA: LAKE DOES NOT EQUAL YES OR NO, BUT = ',
     $ A4)
```

```
      STOP
 1020 IF(SEDLKE.EQ.YES.OR.SEDLKE.EQ.NO)GO TO 1040
      WRITE(IWP,1030)SEDLKE
 1030 FORMAT(1X,'ERROR IN DATA: SEDLKE DOES NOT EQUAL YES OR NO, BUT = '
     $, A4)
      STOP
 1040 IF(TRICON.EQ.YES.OR.TRICON.EQ.NO)GO TO 1060
      WRITE(IWP,1050)TRICON
 1050 FORMAT(1X,'ERROR IN DATA: TRICON DOES NOT EQUAL YES OR NO, BUT = '
     $, A4)
      STOP
 1060 CONTINUE
      IF(SEDLKE.EQ.NO)GO TO 13
      WRITE(IWP,11)
 11   FORMAT(37X,'YES',5X,'SEDLKE',5X,'SIGNIFIES THAT SEDIMENT CONCENTRA
     $TIONS FOR THE LAKE')
      WRITE(IWP,12)
 12   FORMAT(57X,'ARE INPUT (SEE BELOW)')
      GO TO 25
 13   IF(TRICON.EQ.NO)GO TO 19
      WRITE(IWP,14)
 14   FORMAT(38X,'NO',5X,'SEDLKE',5X,'SEDLKE = NO AND TRICON = YES SIGNI
     $FY THAT SEDIMENT')
      WRITE(IWP,16)
 16   FORMAT(37X,'YES',5X,'TRICON',6X,'CONCENTRATIONS FOR A TRIBUTARY FL
     $OWING INTO A LAKE')
      WRITE(IWP,18)
 18   FORMAT(57X,'ARE INPUT (SEE BELOW)')
      GO TO 25
 19   WRITE(IWP,21)
 21   FORMAT(38X,'NO',5X,'SEDLKE',5X,'SEDLKE = NO AND TRICON = NO SIGNIF
     $Y THAT SEDIMENT')
      WRITE(IWP,23)
 23   FORMAT(38X,'NO',5X,'TRICON',6X,'PARAMETERS (FOR LAURSENS FORMULA)
     $FOR A TRIBUTARY')
      WRITE(IWP,24)
 24   FORMAT(57X,'FLOWING INTO A LAKE ARE INPUT (SEE BELOW)')
C
C
 25   IF(RIVER.EQ.YES)WRITE(IWP,26)
 26   FORMAT(37X,'YES',6X,'RIVER',5X,'SIGNIFIES THAT A RIVER IS BEING CO
     $NSIDERED')
      IF(RIVER.EQ.NO)WRITE(IWP,27)
 27   FORMAT(38X,'NO',6X,'RIVER',5X,'SIGNIFIES THAT A RIVER IS NOT BEING
     $ CONSIDERED')
      IF(RIVER.EQ.NO)GO TO 41
      IF(RIVER.EQ.YES)GO TO 1120
      WRITE(IWP,1110)RIVER
 1110 FORMAT(1X,'ERROR IN DATA: RIVER DOES NOT EQUAL YES OR NO, BUT = '
     $, A4)
      STOP
 1120 IF(SEDRIV.EQ.YES.OR.SEDRIV.EQ.NO)GO TO 1140
      WRITE(IWP,1130)SEDRIV
 1130 FORMAT(1X,'ERROR IN DATA: SEDRIV DOES NOT EQUAL YES OR NO, BUT = '
     $, A4)
      STOP
 1140 CONTINUE
      IF(SEDRIV.EQ.NO)GO TO 37
      WRITE(IWP,28)
 28   FORMAT(37X,'YES',5X,'SEDRIV',5X,'SIGNIFIES THAT SEDIMENT CONCENTRA
     $TIONS FOR THE')
      WRITE(IWP,29)
 29   FORMAT(57X,'RIVER ARE INPUT (SEE BELOW)')
      GO TO 41
 37   WRITE(IWP,38)
 38   FORMAT(38X,'NO',5X,'SEDRIV',5X,'SIGNIFIES THAT SEDIMENT PARAMETERS
     $ (FOR LAURSENS')
      WRITE(IWP,39)
 39   FORMAT(57X,'FORMULA) FOR THE RIVER ARE INPUT (SEE BELOW)')
C
C
 41   IF(ESTU.EQ.YES)WRITE(IWP,42)
 42   FORMAT(37X,'YES',6X,'ESTU',6X,'SIGNIFIES THAT AN ESTUARY IS BEING
     $CONSIDERED')
      IF(ESTU.EQ.NO)WRITE(IWP,43)
 43   FORMAT(38X,'NO',6X,'ESTU',6X,'SIGNIFIES THAT AN ESTUARY IS NOT BEI
     $NG CONSIDERED')
      IF(ESTU.EQ.NO)GO TO 51
      IF(ESTU.EQ.YES)GO TO 1220
      WRITE(IWP,1210)ESTU
 1210 FORMAT(1X,'ERROR IN DATA: ESTU DOES NOT EQUAL YES OR NO, BUT = '
     $ ,A4)
      STOP
 1220 IF(DISFLG.EQ.YES.OR.DISFLG.EQ.NO)GO TO 1240
      WRITE(IWP,1230)DISFLG
 1230 FORMAT(1X,'ERROR IN DATA: DISFLG DOES NOT EQUAL YES OR NO, BUT = '
     $, A4)
      STOP
 1240 CONTINUE
      IF(DISFLG.EQ.NO)GO TO 46
      WRITE(IWP,44)
 44   FORMAT(37X,'YES',5X,'DISFLG',5X,'S"GNIFIES THAT THE LONGITUDINAL D
     $ISPERSION')
      WRITE(IWP,45)
 45   FORMAT(57X,'COEFFICIENT (FOR ESTUARY) IS INPUT (SEE BELOW)')
      GO TO 51
 46   WRITE(IWP,47)
 47   FORMAT(38X,'NO',5X,'DISFLG',5X,'SIGNIFIES THAT THE MAXIMUM TIDAL V
     $ELOCITY, USED TO')
      WRITE(IWP,48)
 48   FORMAT(57X,'CALCULATE THE LONGITUDINAL DISPERSION COEFFICIENT, IS
     $INPUT (SEE BELOW)')
C
C
 51   IF(OCEAN.EQ.YES)WRITE(IWP,53)
 53   FORMAT(37X,'YES',6X,'OCEAN',5X,'SIGNIFIES THAT AN OCEAN IS BEING C
     $ONSIDERED')
      IF(OCEAN.EQ.NO)WRITE(IWP,54)
 54   FORMAT(38X,'NO',6X,'OCEAN',5X,'SIGNIFIES THAT AN OCEAN IS NOT BEIN
     $G CONSIDERED')
      IF(OCEAN.EQ.YES.OR.OCEAN.EQ.NO)GO TO 1320
      WRITE(IWP,1310)OCEAN
 1310 FORMAT(1X,'ERROR IN DATA: OCEAN DOES NOT EQUAL YES OR NO, BUT = '
     $,A4)
      STOP
 1320 CONTINUE
C
C
      IF(WATBOD.EQ.NO)GO TO 57
      IF(CHMFLG.EQ.ACID.OR.CHMFLG.EQ.BASE.OR.CHMFLG.EQ.NONE)GO TO 1340
      WRITE(IWP,1330)CHMFLG
 1330 FORMAT(1X,'ERROR IN DATA: CHMFLG DOES NOT EQUAL ACID OR BASE OR NO
     $NE, BUT = ',A4)
      STOP
 1340 CONTINUE
      IF(CHMFLG.EQ.ACID)WRITE(IWP,55)
 55   FORMAT(36X,'ACID',5X,'CHMFLG',5X,'SIGNIFIES THAT CHEMICAL IS AN AC
     $ID')
      IF(CHMFLG.EQ.BASE)WRITE(IWP,56)
 56   FORMAT(36X,'BASE',5X,'CHMFLG',5X,'SIGNIFIES THAT CHEMICAL IS A BAS
     $E')
      IF(CHMFLG.EQ.NONE)WRITE(IWP,58)
 58   FORMAT(36X,'NONE',5X,'CHMFLG',5X,'SIGNIFIES THAT CHEMICAL IS NEUTR
     $AL')
 57   CONTINUE
C
      IF(OCEAN.EQ.YES.AND.LAKE.EQ.NO.AND.RIVER.EQ.NO.AND.ESTU.EQ.NO)
     $   GO TO 100
C
      WRITE(IWP,15)
 15   FORMAT('0',//,51X,'AIR COMPARTMENT PARAMETERS INPUT')
      WRITE(IWP,17)
 17   FORMAT('0',15X,'DEFINITION',20X,'NAME',9X,'UNIT',6X,'VALUE(S)',/)
      DO 30 IYR=1,JYRS
      READ(IRA,20) (UW(MON,IYR),MON=1,6)
   20 FORMAT(20X,6E10.3)
      WRITE(IWP,22)IYR,(UW(MON,IYR),MON=1,6)
 22   FORMAT(10X,'WIND SPEED FOR MON=1, 6 IYR=',I2,3X,'UW(MON,IYR)'5X,
     $'M/S',5X,6(1PE10.3,1X))
      READ(IRA,20) (UW(MON,IYR),MON=7,12)
 30   WRITE(IWP,31)IYR,(UW(MON,IYR),MON=7,12)
 31   FORMAT(25X,'MON=7,12 IYR=',I2,27X,6(1PE10.3,1X))
      READ(IRA,20) UDG,WRATG,AK
      WRITE(IWP,32)UDG
 32   FORMAT(7X,'DRY DEPOSITION VELOCITY FOR GASES',7X,'UDG',9X,'M/S',
     $5X,1PE10.3)
      WRITE(IWP,33)WRATG
 33   FORMAT(17X,'WASHOUT RATIO FOR GASES',6X,'WRATG',8X,'(-)',5X,
     $1PE10.3)
      WRITE(IWP,34)AK
 34   FORMAT(11X,'AIR CHEMICAL DEGRADATION RATE',7X,'AK',9X,'S**-1',4X,
     $1PE10.3)
      IF(AIRFLG.EQ.NONE) GO TO 100
      DO 35 IYR=1,JYRS
      READ(IRA,20) (QS(MON,IYR),MON=1,6)
      WRITE(IWP,36)IYR,(QS(MON,IYR),MON=1,6)
 36   FORMAT(2X,'AIR POLLUTANT RATE FOR MON=1, 6 IYR=',I2,3X,
     $'QS(MON,IYR)',5X,'KG/S',4X,6(1PE10.3,1X))
```

```
      READ(IRA,20) (QS(MON,IYR),MON=7,12)
 35   WRITE(IWP,31)IYR,(QS(MON,IYR),MON=7,12)
      IF(AIRFLG.EQ.AREA) GO TO 70
      IF(AIRFLG.EQ.POINT) GO TO 50
      WRITE(IWP,40) AIRFLG
   40 FORMAT(1X,'ERROR IN DATA: AIRFLG DOES NOT EQUAL NONE,AREA, OR POIN
     $T, BUT = ',A4)
      STOP
   50 DO 60 IYR=1,JYRS
      READ(IRA,20) (HMIX(MON,IYR),MON=1,6)
      WRITE(IWP,52)IYR,(HMIX(MON,IYR),MON=1,6)
 52   FORMAT(7X,'MIXING HEIGHT FOR MON=1, 6 IYR=',I2,2X,'HMIX(MON,IYR)',
     $5X,'M',6X,6(1PE10.3,1X))
      READ(IRA,20) (HMIX(MON,IYR),MON=7,12)
 60   WRITE(IWP,31)IYR,(HMIX(MON,IYR),MON=7,12)
      READ(IRA,20) HS,VG,VS,SRAD,RHO,ENTPY
      WRITE(IWP,61)HS
 61   FORMAT(28X,'STACK HEIGHT',7X,'HS',11X,'M',6X,1PE10.3)
      WRITE(IWP,62)VG
 62   FORMAT(9X,'GRAVITATIONAL SETTLING VELOCITY',7X,'VG',10X,'M/S',
     $5X,1PE10.3)
      WRITE(IWP,63)VS
 63   FORMAT(17X,'STACK GAS EXIT VELOCITY',7X,'VS',10X,'M/S',5X,1PE10.3)
      WRITE(IWP,64)SRAD
 64   FORMAT(28X,'STACK RADIUS',6X,'SRAD',10X,'M',6X,1PE10.3)
      WRITE(IWP,65)RHO
 65   FORMAT(23X,'STACK GAS DENSITY',7X,'RHO',8X,'KG/M**3',2X,1PE10.3)
      WRITE(IWP,66)ENTPY
 66   FORMAT(19X,'ENTHALPY OF STACK GAS',6X,'ENTPY',8X,'J/KG',4X,
     $1PE10.3)
      GO TO 80
C
   70 READ(IRA,20) CTYLTH
      WRITE(IWP,75)CTYLTH
 75   FORMAT(12X,'LENGTH OF CITY OR URBAN AREA',5X,'CTYLTH',9X,'M',
     $6X,1PE10.3)
C
   80 IF(AIRPOL.EQ.PART) GO TO 90
      IF(AIRPOL.EQ.GAS) GO TO 100
      WRITE(IWP,85) AIRPOL
   85 FORMAT(1X,'ERROR IN DATA: AIRPOL DOES NOT EQUAL GAS OR PARTICULATE
     $, BUT = ',A4)
      STOP
   90 READ(IRA,20) UDP,WRATP
      WRITE(IWP,92)UDP
 92   FORMAT(2X,'DRY DEPOSITION VELOCITY (PARTICULATES)',7X,'UDP',9X,
     $'M/S',5X,1PE10.3)
      WRITE(IWP,94)WRATP
 94   FORMAT(10X,'WASHOUT RATIO FOR PARTICULATES',6X,'WRATP',8X,'(-)',
     $5X,1PE10.3)
C
  100 CONTINUE
C
      IF(WATBOD.NE.NO)GO TO 99
      IF(AIRFLG.NE.POINT)GO TO 98
      READ(IRA,20)XLENS
      WRITE(IWP,96)XLENS
 96   FORMAT(2X,'LENGTH OF PLUME CONSIDERED (OVER SOIL)',6X,'XLENS',9X,'
     $M',6X,1PE10.3)
 98   WRITE(IWP,97)
 97   FORMAT('0',//,36X,'NO WATER BODY IS CONSIDERED - SOIL AND AIR INTE
     $RACTION ONLY')
      GO TO 300
C
 99   WRITE(IWP,101)
 101  FORMAT('0',//,50X,'WATER COMPARTMENT PARAMETERS INPUT')
      WRITE(IWP,17)
      READ(IRW,20) DISK
      WRITE(IWP,107)DISK
 107  FORMAT(19X,'DISSOCIATION CONSTANT',6X,'DISK',7X,'MOLES/L',3X,
     $1PE10.3)
C
C
      IF(LAKE.NE.YES) GO TO 150
      WRITE(IWP,113)
 113  FORMAT('0','LAKE :',/)
      DO 110 IYR=1,JYRS
      READ(IRW,20) (WMINL(MON,IYR),MON=1,6)
      WRITE(IWP,114)IYR,(WMINL(MON,IYR),MON=1,6)
 114  FORMAT(5X,'LAKE POLLUTANT RATE MON=1, 6 IYR=',I2,2X,'WMINL(MON,IYR
     $)',3X,'KG/S',4X,6(1PE10.3,1X))
      READ(IRW,20) (WMINL(MON,IYR),MON=7,12)
 110  WRITE(IWP,31)IYR,(WMINL(MON,IYR),MON=7,12)
      DO 120 IYR=1,JYRS
      READ(IRW,20) (WVELL(MON,IYR),MON=1,6)
      WRITE(IWP,115)IYR,(WVELL(MON,IYR),MON=1,6)
 115  FORMAT(5X,'LAKE WATER VELOCITY MON=1, 6 IYR=',I2,2X,'WVELL(MON,IYR
     $)',3X,'M/S',5X,6(1PE10.3,1X))
      READ(IRW,20) (WVELL(MON,IYR),MON=7,12)
 120  WRITE(IWP,31)IYR,(WVELL(MON,IYR),MON=7,12)
      READ(IRW,20) AREALK,WDEPL,XSOIL,HPLUSL
      WRITE(IWP,121)AREALK
 121  FORMAT(20X,'SURFACE AREA OF LAKE',5X,'AREALK',8X,'M**2',4X,
     $1PE10.3)
      WRITE(IWP,122)WDEPL
 122  FORMAT(27X,'DEPTH OF LAKE',6X,'WDEPL',9X,'M',6X,1PE10.3)
      WRITE(IWP,123)XSOIL
 123  FORMAT(7X,'LENGTH OF WATERSHED OUT FROM LAKE',6X,'XSOIL',9X,'M',
     $6X,1PE10.3)
      WVOLL=AREALK*WDEPL
      WRITE(IWP,129)HPLUSL
 129  FORMAT(36X,'[H+]',5X,'HPLUSL',7X,'MOLES/L',2X,1PE10.3)
      READ(IRW,20) WKPL,WKHL,WKOL,WKBL,WKVL,SWKSWL
      WRITE(IWP,102)WKPL
 102  FORMAT(8X,'PHOTOLYSIS RATE CONSTANT (WATER)',6X,'WKPL',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,103)WKHL
 103  FORMAT(8X,'HYDROLYSIS RATE CONSTANT (WATER)',6X,'WKHL',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,104)WKOL
 104  FORMAT(9X,'OXIDATION RATE CONSTANT (WATER)',6X,'WKOL',8X,'S**-1',
     $4X,1PE10.3)
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      WRITE(IWP,105)WKBL
  105 FORMAT(4X,'BIODEGRADATION RATE CONSTANT (WATER)',6X,'WKBL',8X,
     $'S**-1',4X,1PE10.3)
      WRITE(IWP,106)WKVL
  106 FORMAT(4X,'VOLATILIZATION RATE CONSTANT (WATER)',6X,'WKVL',8X,
     $'S**-1',4X,1PE10.3)
      WRITE(IWP,112)SWKSWL
  112 FORMAT(8X,'SOIL-WATER PARTITION COEFFICIENT',5X,'SWKSWL',4X,
     $'MOL/KG/MOL/L',1PE10.3)
C
      IF(SEDLKE.EQ.YES) GO TO 130
      IF(TRICON.EQ.YES) GO TO 130
C
C HERE SEDLKE AND TRICON BOTH EQUAL NO SO MUST INPUT SEDIMENT
C  PARAMETERS FOR TRIBUTARY FLOWING INTO LAKE.
C
      READ(IRW,20) DIASDT,DENSDT,DENWT,WDEPT,SLOPET
      WRITE(IWP,124)DIASDT
  124 FORMAT(3X,'MEDIAN SEDIMENT DIAMETER IN TRIBUTARY',5X,'DIASDT',9X,
     $'MM',5X,1PE10.3)
      WRITE(IWP,125)DENSDT
  125 FORMAT(11X,'SEDIMENT DENSITY IN TRIBUTARY',5X,'DENSDT',7X,'G/CM**3
     $',2X,1PE10.3)
      WRITE(IWP,126)DENWT
  126 FORMAT(14X,'WATER DENSITY IN TRIBUTARY',6X,'DENWT',7X,'G/CM**3',
     $2X,1PE10.3)
      WRITE(IWP,127)WDEPT
  127 FORMAT(22X,'DEPTH OF TRIBUTARY ',5X,'WDEPT',9X,'M',6X,1PE10.3)
      WRITE(IWP,128)SLOPET
  128 FORMAT(22X,'SLOPE OF TRIBUTARY ',4X,'SLOPET',8X,'(-)',5X,1PE10.3)
      GO TO 150
  130 DO 140 IYR=1,JYRS
      READ(IRW,20) (SEDCL(MON,IYR),MON=1,6)
      IF(SEDLKE.EQ.YES)WRITE(IWP,132)IYR,(SEDCL(MON,IYR),MON=1,6)
  132 FORMAT(3X,'SEDIMENT CONC. (LAKE) MON=1, 6 IYR=',I2,2X,'SEDCL(MON,I
     $YR)',2X,'KG/M**3',2X,6(1PE10.3,1X))
      IF(TRICON.EQ.YES)WRITE(IWP,134)IYR,(SEDCL(MON,IYR),MON=1,6)
  134 FORMAT(1X,'SEDIMENT CONC-TRIBUTARY MON=1, 6 IYR=',I2,2X,'SEDCL(MON
     $,IYR)',2X,'KG/M**3',2X,6(1PE10.3,1X))
      READ(IRW,20) (SEDCL(MON,IYR),MON=7,12)
  140 WRITE(IWP,31)IYR,(SEDCL(MON,IYR),MON=7,12)
C
C
  150 IF(RIVER.NE.YES) GO TO 200
      WRITE(IWP,152)
  152 FORMAT('0','RIVER :',/)
      DO 160 IYR=1,JYRS
      READ(IRW,20) (WMINR(MON,IYR),MON=1,6)
      WRITE(IWP,154)IYR,(WMINR(MON,IYR),MON=1,6)
  154 FORMAT(4X,'RIVER POLLUTANT RATE MON=1, 6 IYR=',I2,2X,'WMINR(MON,IY
     $R)',3X,'KG/S',4X,6(1PE10.3,1X))
      READ(IRW,20) (WMINR(MON,IYR),MON=7,12)
  160 WRITE(IWP,31)IYR,(WMINR(MON,IYR),MON=7,12)
      DO 170 IYR=1,JYRS
      READ(IRW,20) (WVELR(MON,IYR),MON=1,6)
      WRITE(IWP,162)IYR,(WVELR(MON,IYR),MON=1,6)
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162  FORMAT(4X,'RIVER WATER VELOCITY MON=1, 6 IYR=',I2,2X,'WVELR(MON,IY
    $R)',3X,'M/S',5X,6(1PE10.3,1X))
     READ(IRW,20) (WVELR(MON,IYR),MON=7,12)
170  WRITE(IWP,31)IYR,(WVELR(MON,IYR),MON=7,12)
     READ(IRW,180) NR
 180 FORMAT(28X,I2)
     WRITE(IWP,182)NR
182  FORMAT(23X,'NUMBER OF REACHES',7X,'NR',10X,'(-)',12X,I3)
     READ(IRW,20) WLENR,WWIDR,WDEPR,HPLUSR
     WRITE(IWP,181)WLENR
181  FORMAT(19X,'LENGTH OF RIVER REACH',6X,'WLENR',9X,'M',6X,1PE10.3)
     WRITE(IWP,188)WWIDR
188  FORMAT(20X,'WIDTH OF RIVER REACH',6X,'WWIDR',9X,'M',6X,1PE10.3)
     WRITE(IWP,183)WDEPR
183  FORMAT(20X,'DEPTH OF RIVER REACH',6X,'WDEPR',9X,'M',6X,1PE10.3)
     WVOLR=WLENR*WWIDR*WDEPR
     WRITE(IWP,189)HPLUSR
189  FORMAT(36X,'[H+]',5X,'HPLUSR',7X,'MOLES/L',2X,1PE10.3)
     READ(IRW,20) WKPR,WKHR,WKOR,WKBR,WKVR,SWKSWR
     WRITE(IWP,191)WKPR
191  FORMAT(8X,'PHOTOLYSIS RATE CONSTANT (WATER)',6X,'WKPR',8X,'S**-1',
    $4X,1PE10.3)
     WRITE(IWP,193)WKHR
193  FORMAT(8X,'HYDROLYSIS RATE CONSTANT (WATER)',6X,'WKHR',8X,'S**-1',
    $4X,1PE10.3)
     WRITE(IWP,194)WKOR
194  FORMAT(9X,'OXIDATION RATE CONSTANT (WATER)',6X,'WKOR',8X,'S**-1',
    $4X,1PE10.3)
     WRITE(IWP,196)WKBR
196  FORMAT(4X,'BIODEGRADATION RATE CONSTANT (WATER)',6X,'WKBR',8X,
    $'S**-1',4X,1PE10.3)
     WRITE(IWP,197)WKVR
197  FORMAT(4X,'VOLATILIZATION RATE CONSTANT (WATER)',6X,'WKVR',8X,
    $'S**-1',4X,1PE10.3)
     WRITE(IWP,198)SWKSWR
198  FORMAT(8X,'SOIL-WATER PARTITION COEFFICIENT',5X,'SWKSWR',4X,
    $'MOL/KG/MOL/L',1PE10.3)
     IF(SEDRIV.EQ.YES) GO TO 190
     READ(IRW,20) DIASDR,DENSDR,DENWR,SLOPER
     WRITE(IWP,184)DIASDR
184  FORMAT(7X,'MEDIAN SEDIMENT DIAMETER IN RIVER',5X,'DIASDR',9X,'MM',
    $5X,1PE10.3)
     WRITE(IWP,185)DENSDR
185  FORMAT(15X,'SEDIMENT DENSITY IN RIVER',5X,'DENSDR',7X,'G/CM**3',
    $2X,1PE10.3)
     WRITE(IWP,186)DENWR
186  FORMAT(18X,'WATER DENSITY IN RIVER',6X,'DENWR',7X,'G/CM**3',2X,
    $1PE10.3)
     WRITE(IWP,187)SLOPER
187  FORMAT(26X,'SLOPE OF RIVER',5X,'SLOPER',8X,'(-)',5X,1PE10.3)
     GO TO 200
 190 DO 195 IYR=1,JYRS
     READ(IRW,20) (SEDCR(MON,IYR),MON=1,6)
     WRITE(IWP,192)IYR,(SEDCR(MON,IYR),MON=1,6)
192  FORMAT(2X,'SEDIMENT CONC. (RIVER) MON=1, 6 IYR=',I2,2X,
    $'SEDCR(MON,IYR)',2X,'KG/M**3',2X,6(1PE10.3))
```

```
      READ(IRW,20) (SEDCR(MON,IYR),MON=7,12)
  195 WRITE(IWP,31)IYR,(SEDCR(MON,IYR),MON=7,12)
C
C
  200 IF(ESTU.NE.YES) GO TO 250
      WRITE(IWP,202)
  202 FORMAT('0','ESTUARY :',/)
      DO 210 IYR=1,JYRS
      READ(IRW,20) (WMINE(MON,IYR),MON=1,6)
      WRITE(IWP,204)IYR,(WMINE(MON,IYR),MON=1,6)
  204 FORMAT(2X,'ESTUARY POLLUTANT RATE MON=1, 6 IYR=',I2,2X,'WMINE(MON,
     $IYR)',3X,'KG/S',4X,6(1PE10.3,1X))
      READ(IRW,20) (WMINE(MON,IYR),MON=7,12)
  210 WRITE(IWP,31)IYR,(WMINE(MON,IYR),MON=7,12)
      DO 220 IYR=1,JYRS
      READ(IRW,20) (WVELE(MON,IYR),MON=1,6)
      WRITE(IWP,212)IYR,(WVELE(MON,IYR),MON=1,6)
  212 FORMAT(4X,'FRESH WATER VELOCITY MON=1, 6 IYR=',I2,2X,'WVELE(MON,IY
     $R)',3X,'M/S',5X,6(1PE10.3,1X))
      READ(IRW,20) (WVELE(MON,IYR),MON=7,12)
  220 WRITE(IWP,31)IYR,(WVELE(MON,IYR),MON=7,12)
      READ(IRW,180) NPTSE
      WRITE(IWP,222)NPTSE
  222 FORMAT(1X,'# PTS UP & DOWNSTREAM OF SOURCE(OUTPUT)',6X,'NPTSE',
     $8X,'(-)',12X,I3)
      READ(IRW,20) WLENE,WWIDE,WDEPE,EL,TIDMAX,HPLUSE
      WRITE(IWP,223)WLENE
  223 FORMAT(23X,'LENGTH OF ESTUARY',6X,'WLENE',9X,'M',6X,1PE10.3)
      WRITE(IWP,224)WWIDE
  224 FORMAT(24X,'WIDTH OF ESTUARY',6X,'WWIDE',9X,'M',6X,1PE10.3)
      WRITE(IWP,225)WDEPE
  225 FORMAT(24X,'DEPTH OF ESTUARY',6X,'WDEPE',9X,'M',6X,1PE10.3)
      IF(DISFLG.EQ.YES)WRITE(IWP,226)EL
  226 FORMAT(5X,'LONGITUDINAL DISPERSION COEFFICIENT',7X,'EL',9X,
     $'M**2/S',3X,1PE10.3)
      IF(DISFLG.EQ.NO)WRITE(IWP,227)TIDMAX
  227 FORMAT(18X,'MAXIMUM TIDAL VELOCITY',5X,'TIDMAX',8X,'M/S',5X,
     $1PE10.3)
      WRITE(IWP,229)HPLUSE
  229 FORMAT(36X,'[H+]',5X,'HPLUSE',7X,'MOLES/L',2X,1PE10.3)
      READ(IRW,20) WKPE,WKHE,WKOE,WKBE,WKVE,SWKSWE
      WRITE(IWP,231)WKPE
  231 FORMAT(8X,'PHOTOLYSIS RATE CONSTANT (WATER)',6X,'WKPE',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,232)WKHE
  232 FORMAT(8X,'HYDROLYSIS RATE CONSTANT (WATER)',6X,'WKHE',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,233)WKOE
  233 FORMAT(9X,'OXIDATION RATE CONSTANT (WATER)',6X,'WKOE',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,234)WKBE
  234 FORMAT(4X,'BIODEGRADATION RATE CONSTANT (WATER)',6X,'WKBE',8X,
     $'S**-1',4X,1PE10.3)
      WRITE(IWP,235)WKVE
  235 FORMAT(4X,'VOLATILIZATION RATE CONSTANT (WATER)',6X,'WKVE',8X,
     $'S**-1',4X,1PE10.3)
```

```
      WRITE(IWP,236)SWKSWE
  236 FORMAT(8X,'SOIL-WATER PARTITION COEFFICIENT',5X,'SWKSWE',4X,
     $'MOL/KG/MOL/L',1PE10.3)
C
      DO 230 IYR=1,JYRS
      READ(IRW,20) (SEDCE(MON,IYR),MON=1,6)
      WRITE(IWP,228)IYR,(SEDCE(MON,IYR),MON=1,6)
  228 FORMAT(1X,'SEDIMENT CONC.(ESTUARY) MON=1, 6 IYR=',I2,2X,'SEDCE(MON
     $,IYR)',2X,'KG/M**3',2X,6(1PE10.3,1X))
      READ(IRW,20) (SEDCE(MON,IYR),MON=7,12)
  230 WRITE(IWP,31)IYR,(SEDCE(MON,IYR),MON=7,12)
C
C
  250 IF(OCEAN.NE.YES) GO TO 300
      WRITE(IWP,252)
  252 FORMAT('0','OCEAN :',/)
      DO 260 IYR=1,JYRS
      READ(IRW,20) (WCINO(MON,IYR),MON=1,6)
      WRITE(IWP,254)IYR,(WCINO(MON,IYR),MON=1,6)
  254 FORMAT(2X,'0.02*CONC. OF EFFLUENT MON=1, 6 IYR=',I2,2X,
     $'WCINO(MON,IYR)',2X,'KG/M**3',2X,6(1PE10.3,1X))
      READ(IRW,20) (WCINO(MON,IYR),MON=7,12)
  260 WRITE(IWP,31)IYR,(WCINO(MON,IYR),MON=7,12)
      DO 270 IYR=1,JYRS
      READ(IRW,20) (WVELO(MON,IYR),MON=1,6)
      WRITE(IWP,262)IYR,(WVELO(MON,IYR),MON=1,6)
  262 FORMAT(2X,'OCEAN CURRENT VELOCITY MON=1, 6 IYR=',I2,2X,
     $'WVELO(MON,IYR)',3X,'M/S',5X,6(1PE10.3,1X))
      READ(IRW,20) (WVELO(MON,IYR),MON=7,12)
  270 WRITE(IWP,31)IYR,(WVELO(MON,IYR),MON=7,12)
      READ(IRW,20) BO,XOCEAN,HPLUSO
      WRITE(IWP,276)BO
  276 FORMAT(19X,'LENGTH OF LINE SOURCE',7X,'BO',11X,'M',6X,1PE10.3)
      WRITE(IWP,278)XOCEAN
  278 FORMAT(1X,'DISTANCE BETWEEN POINTS IN OCEAN OUTPUT',5X,'XOCEAN',9X
     $,'M',6X,1PE10.3)
      WRITE(IWP,277)HPLUSO
  277 FORMAT(36X,'[H+]',5X,'HPLUSO',7X,'MOLES/L',2X,1PE10.3)
      READ(IRW,20) WKPO,WKHO,WKOO,WKBO,WKVO,SWKSWO
      WRITE(IWP,290)WKPO
  290 FORMAT(8X,'PHOTOLYSIS RATE CONSTANT (WATER)',6X,'WKPO',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,291)WKHO
  291 FORMAT(8X,'HYDROLYSIS RATE CONSTANT (WATER)',6X,'WKHO',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,292)WKOO
  292 FORMAT(9X,'OXIDATION RATE CONSTANT (WATER)',6X,'WKOO',8X,'S**-1',
     $4X,1PE10.3)
      WRITE(IWP,293)WKBO
  293 FORMAT(4X,'BIODEGRADATION RATE CONSTANT (WATER)',6X,'WKBO',8X,
     $'S**-1',4X,1PE10.3)
      WRITE(IWP,294)WKVO
  294 FORMAT(4X,'VOLATILIZATION RATE CONSTANT (WATER)',6X,'WKVO',8X,
     $'S**-1',4X,1PE10.3)
      WRITE(IWP,295)SWKSWO
  295 FORMAT(8X,'SOIL-WATER PARTITION COEFFICIENT',5X,'SWKSWO',4X,
     $'MOL/KG/MOL/L',1PE10.3)
      READ(IRW,180)NPTSO
      WRITE(IWP,279)NPTSO
  279 FORMAT(3X,'NUMBER OF POINTS FROM SOURCE (OUTPUT)',6X,'NPTSO',8X,'(
     $-)',12X,I3)
C
      DO 280 IYR=1,JYRS
      READ(IRW,20) ( SEDCO(MON,IYR),MON=1,6)
      WRITE(IWP,282)IYR,(SEDCO(MON,IYR),MON=1,6)
  282 FORMAT(2X,'SEDIMENT CONC. (OCEAN) MON=1, 6 IYR=',I2,2X,'SEDCO(MON,
     $IYR)',2X,'KG/M**3',2X,6(1PE10.3,1X))
      READ(IRW,20) (SEDCO(MON,IYR),MON=7,12)
  280 WRITE(IWP,31)IYR,(SEDCO(MON,IYR),MON=7,12)
C
  999 CONTINUE
  300 CONTINUE
      WRITE(IWG,310)
  310 FORMAT('1',61X,'SCENARIO',//)
      WRITE(IWG,320)
  320 FORMAT('0',54X,'TYPE OF SOURCE TERMS',/)
C
      IF(AIRFLG.EQ.POINT)WRITE(IWG,330)
  330 FORMAT(1X,57X,'AIR         - POINT',//)
      IF(AIRFLG.EQ.AREA)WRITE(IWG,340)
  340 FORMAT(1X,57X,'AIR         - AREA',//)
      IF(AIRFLG.EQ.NONE)WRITE(IWG,350)
  350 FORMAT(1X,57X,'AIR         - NONE',//)
C
      WRITE(IWG,360)
  360 FORMAT(1X,57X,'WATER BODY(IES) CONSIDERED:')
      IF(WATBOD.EQ.NO)WRITE(IWG,361)
  361 FORMAT(69X,'- NONE')
      IF(WATBOD.EQ.NO)GO TO 420
C
C
      IF(LAKE.NE.YES)GO TO 385
      DO 365 IYR=1,JYRS
      DO 365 MON=1,12
  365 IF(WMINL(MON,IYR).NE.0.0)GO TO 375
      WRITE(IWG,370)
  370 FORMAT(1X,68X,'- LAKE (NO SOURCE)')
      GO TO 385
  375 ILAKE=1
      WRITE(IWG,380)
  380 FORMAT(1X,68X,'- LAKE (HAS SOURCE)')
C
C
  385 IF(RIVER.NE.YES)GO TO 400
      DO 390 IYR=1,JYRS
      DO 390 MON=1,12
  390 IF(WMINR(MON,IYR).NE.0.0)GO TO 395
      WRITE(IWG,392)
  392 FORMAT(1X,68X,'- RIVER (NO SOURCE)')
      GO TO 400
  395 IRIV=1
      WRITE(IWG,397)
  397 FORMAT(1X,68X,'- RIVER (HAS SOURCE)')
C
C
  400 IF(ESTU.NE.YES)GO TO 415
      DO 405 IYR=1,JYRS
      DO 405 MON=1,12
  405 IF(WMINE(MON,IYR).NE.0.0)GO TO 410
      WRITE(IWG,407)
  407 FORMAT(1X,68X,'- ESTUARY (NO SOURCE)')
      GO TO 415
  410 IEST=1
      WRITE(IWG,412)
  412 FORMAT(1X,68X,'- ESTUARY (HAS SOURCE)')
C
C
  415 IF(OCEAN.NE.YES)GO TO 420
      DO 416 IYR=1,JYRS
      DO 416 MON=1,12
  416 IF(WCINO(MON,IYR).NE.0.0)GO TO 418
      WRITE(IWG,417)
  417 FORMAT(1X,68X,'- OCEAN (NO SOURCE)')
      GO TO 420
  418 IOCN=1
      WRITE(IWG,419)
  419 FORMAT(1X,68X,'- OCEAN (HAS SOURCE)')
C
  420 DO 422 MON=1,12
  422 IF(RUNM1(4,MON).NE.0.0)GO TO 430
      WRITE(IWG,425)
  425 FORMAT('0',57X,'UPPER SOIL - NONE')
      GO TO 450
  430 IUPSL=1
      WRITE(IWG,440)
  440 FORMAT('0',57X,'UPPER SOIL - DIRECT APPLICATION')
  450 DO 452 MON=1,12
  452 IF(RUNM1(5,MON).NE.0.0)GO TO 456
      WRITE(IWG,454)
  454 FORMAT(58X,'MIDDLE SOIL - NONE')
      GO TO 458
  456 IMSL=1
      WRITE(IWG,457)
  457 FORMAT(58X,'MIDDLE SOIL - DIRECT APPLICATION')
  458 DO 460 MON=1,12
  460 IF(RUNM1(6,MON).NE.0.0)GO TO 480
      WRITE(IWG,470)
  470 FORMAT(58X,'LOWER SOIL - NONE')
      GO TO 500
  480 ILSL=1
      WRITE(IWG,490)
  490 FORMAT(58X,'LOWER SOIL - DIRECT APPLICATION')
C
  500 WRITE(IWG,510)(TITLES(1,IR),IR=1,12)
  510 FORMAT('0',//,55X,'GEOGRAPHIC REGION - ',12A4,//)
      WRITE(IWG,520)
  520 FORMAT('0',54X,'MAGNITUDE OF SOURCE(S)',/)
      WRITE(IWG,530)(AMO(I),I=1,12)
  530 FORMAT(1X,6X,12(6X,A4),/)
      IF(AIRFLG.EQ.NONE)GO TO 580
      WRITE(IWG,540)
  540 FORMAT(3X,'AIR')
      WRITE(IWG,550)
  550 FORMAT(1X,'(KG/SEC)')
      DO 560 IYR=1,JYRS
  560 WRITE(IWG,570)IYR,(QS(MON,IYR),MON=1,12)
  570 FORMAT(2X,'YEAR ',I2,2X,12(1PE9.2,1X))
  580 IF(ILAKE.NE.1)GO TO 620
      WRITE(IWG,590)
  590 FORMAT(/,2X,'LAKE')
      WRITE(IWG,550)
      DO 610 IYR=1,JYRS
  610 WRITE(IWG,570)IYR,(WMINL(MON,IYR),MON=1,12)
  620 IF(IRIV.NE.1)GO TO 650
      WRITE(IWG,630)
  630 FORMAT(/,1X,'RIVER')
      WRITE(IWG,550)
      DO 640 IYR=1,JYRS
  640 WRITE(IWG,570)IYR,(WMINR(MON,IYR),MON=1,12)
  650 IF(IEST.NE.1)GO TO 680
      WRITE(IWG,660)
  660 FORMAT(/,1X,'ESTUARY')
      WRITE(IWG,550)
      DO 670 IYR=1,JYRS
  670 WRITE(IWG,570)IYR,(WMINE(MON,IYR),MON=1,12)
  680 IF(IOCN.NE.1)GO TO 720
      WRITE(IWG,690)
  690 FORMAT(/,1X,'OCEAN')
      WRITE(IWG,700)
  700 FORMAT(1X,'(KG/M**3)')
      DO 710 IYR=1,JYRS
  710 WRITE(IWG,570)IYR,(WCINO(MON,IYR),MON=1,12)
  720 CONTINUE
      IF(IUPSL.NE.1)GO TO 750
      WRITE(IWG,730)
  730 FORMAT(/,1X,'UPPER SOIL')
      WRITE(IWG,740)
  740 FORMAT(1X,'(UG/MON)')
      IYR=1
      WRITE(IWG,570)IYR,(RUNM1(4,MON),MON=1,12)
  750 IF(IMSL.NE.1)GO TO 758
      WRITE(IWG,752)
  752 FORMAT(/,1X,'MIDDLE SOIL')
      WRITE(IWG,740)
      IYR=1
      WRITE(IWG,570)IYR,(RUNM1(5,MON),MON=1,12)
  758 IF(ILSL.NE.1)RETURN
      WRITE(IWG,760)
  760 FORMAT(/,1X,'LOWER SOIL')
      WRITE(IWG,740)
      IYR=1
      WRITE(IWG,570)IYR,(RUNM1(6,MON),MON=1,12)
      RETURN
      END
      SUBROUTINE SEDCON(IMON,IYR)
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $       ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/WPARL/WVELL(12,10),WMINL(12,10),WMTLKE,AREALK,
     $       WDEPL,WVOLL
      COMMON/WPARR/WVELR(12,10),WMINR(12,10),WMTRIV(20),
     $       NR,WWIDR,WLENR,WDEPR,WVOLR,WMTOLD,AREAR
      COMMON/SDPARR/SEDCR(12,10),DIASDR,DENSDR,DENWR,SLOPER,CONSDR
      COMMON/SDPARL/SEDCL(12,10),DIASDT,DENSDT,DENWT,SLOPET,WDEPT,CONSDL
      REAL LAKE,NO
      DIMENSION VDQ(20),PDAT(20),BP(20),CP(20),DP(20)
C
C VDQ, PDAT, BP, CP, DP NEEDED FOR COMPUTING TRAPPING EFFICIENCY P FOR LAKES
C
      DATA VDQ/.002,.003,.005,.007,.01,.02,.03,.05,.07,.1,.2,
     $ .3,.5,.7,1.,2.,3.,5.,7.,10./
      DATA PDAT/.02,.14,.27,.355,.448,.60,.690,.775,.825,.865,.925,
     $ .945,.965,.975,.980,.990,.990,.990,.990,.990/
      DATA BP/146.8928,95.64891,47.32103,37.56698,25.43354,
     $ 9.952678,7.355743,2.710186,2.053512,.9171595,.339577,
     $ .1245326,.07365036,.03086593,.01019481,.005425183,
     $ -.001895546,.0005229092,-.0001960909,.0001960909/
      DATA CP/-29434.42,-21809.42,-2354.518,-2522.503,-1521.977,
     $ -26.10996,-233.5836,1.305765,-34.13947,-3.73896,-2.036866,
     $ -.113578,-.1408333,-.0730889,.004185188,-.00895482,
     $ .001634091,-.0004248637,.00006536365,.00006536365/
      DATA DP/2541667.,3242484.,-27997.51,111169.6,49862.22,
     $ -6915.788,3914.823,-590.7538,337.7834,5.673646,
     $ 6.410959,-.04542552,.1129073,.0858601,-.004380003,.003529637,
     $ -.0003431592,.00008170456,0.,0./
      DATA NO/4H  NO/,IWP/13/
      MON=IMON
      IF(SEDRIV.NE.NO.OR.RIVER.EQ.NO)GO TO 200
 10   IF(MON.GT.1.OR.IYR.GT.1)GO TO 100
C
C THE FOLLOWING COMPUTES THE SEDIMENT CONCENTRATION FOR A
C RIVER OR STREAM. 1ST, COMPUTE LAURSENS FUNCTION.
C
      CALL FUNLAU(DIASDR,DENSDR,DENWR,WDEPR,SLOPER,
     $      TCRITR,FUNCR,TOPFCR,RATIOR)
 100  TOPRIM=TOPFCR*(WVELR(MON,IYR)**2)
      IF((TOPRIM/TCRITR).GT.1.0)GO TO 150
      WRITE(IWP,125)
 125  FORMAT(1X,'STOP IN SEDCON (IN RIVER CALCULATION):  TOPRIM/TCRITR I
     $S < 1.0 CAUSING SEDIMENT CONCENTRATION TO BE NEGATIVE. USER SHOULD
     $ CHECK INPUT DATA FOR ERRORS. IF NO ERRORS, USER SHOULD SET SEDRIV
     $ TO YES AND INPUT EMPIRICAL (GENERIC) DATA (PARAMETER SEDCR(MON,IY
     $R))')
      STOP
C
C HERE CONSDR IS SEDIMENT CONCENTRATION (% BY WEIGHT) (LAURSENS FORMULA)
C
 150  CONSDR=RATIOR*((TOPRIM/TCRITR)-1.0)*FUNCR
C
C CALCULATE CONSDR IN KG/M**3
C
```

```
      CONSDR=CONSDR/((CONSDR/DENSDR)+((100.0-CONSDR)/DENWR))
C
C
C THE FOLLOWING COMPUTES THE SEDIMENT CONCENTRATION FOR A LAKE.
C
 200  CONTINUE
      IF(SEDLKE.NE.NO.OR.LAKE.EQ.NO)RETURN
      IF(TRICON.EQ.NO)GO TO 225
C
C HERE, CONSDL IS SEDIMENT CONCENTRATION FOR TRIBUTARY FLOWING INTO
C A LAKE.
C
      CONSDL=SEDCL(MON,IYR)
      GO TO 245
 225  IF(MON.GT.1.OR.IYR.GT.1)GO TO 230
C
C CALCULATE SEDIMENT CONCENTRATION FOR TRIBUTARY FLOWING INTO LAKE.
C 1ST, COMPUTE LAURSEN'S FUNCTION USING TRIBUTARY PARAMETERS.
C
      CALL FUNLAU(DIASDT,DENSDT,DENWT,WDEPT,SLOPET,TCRITT,FUNCT,
     $            TOPFCT,RATIOT)
 230  TOPRIM=TOPFCT*(WVELL(MON,IYR)**2)
      IF((TOPRIM/TCRITT).GT.1.0)GO TO 240
      WRITE(IWP,235)
 235  FORMAT(1X,'STOP IN SEDCON (IN LAKE CALCULATION):   TOPRIM/TCRIT IS
     $ < 1.0 CAUSING SEDIMENT CONCENTRATION TO BE NEGATIVE. USER SHOULD
     $CHECK INPUT DATA FOR ERRORS. IF NO ERRORS, USER SHOULD SET SEDLKE
     $TO YES AND INPUT EMPIRICAL (GENERIC) DATA (PARAMETER SEDCL(MON,IYR
     $))')
      STOP
C
C HERE CONSDL IS SEDIMENT CONCENTRATION (% BY WEIGHT). (LAURSENS FORMULA)
C
 240  CONSDL=RATIOT*((TOPRIM/TCRITT)-1.0)*FUNCT
C
C CALCULATE CONSDL IN KG/M**3
C
      CONSDL=CONSDL/((CONSDL/DENSDT)+((100.0-CONSDL)/DENWT))
 245  CONTINUE
C
C HERE, NEED MEAN TRIBUTARY FLOW VELOCITY (MONTHLY) AND LENGTH OF
C LAKE TO COMPUTE VOLUME OF LAKE/FLOW RATE (IN S)
C
 250  VOLFLO=SQRT(AREALK)/WVELL(MON,IYR)
C
C CONVERT VOLFLO TO YEARS
C
      VOLFLO=VOLFLO/3.1536E+7
      IF(VOLFLO.LT..002.OR.VOLFLO.GT.10.0)GO TO 300
C
C CALCULATE TRAPPING EFFICIENCY P USING SPLINE
C
      P=SPLEVA(20,VOLFLO,VDQ,PDAT,BP,CP,DP)
      GO TO 400
 300  IF(VOLFLO.LT..002)P=0.0
      IF(VOLFLO.GT.10.0)P=.99
```

```
C
C COMPUTE SEDIMENT CONCENTRATION IN LAKE CONSDL IN KG/M**3.
C
 400  CONSDL=CONSDL*(1.0-P)
      RETURN
      END
      FUNCTION SPLEVA(NPTS,U,X,Y,B,C,D)
      DIMENSION X(NPTS),Y(NPTS),B(NPTS),C(NPTS),D(NPTS)
      DATA I/1/
C
C THIS SUBROUTINE EVALUATES A CUBIC SPLINE FUNCTION USING
C HORNER'S RULE.
C
C NPTS=# OF DATA POINTS
C U=ABSCISSA AT WHICH SPLINE IS TO BE EVALUATED
C X,Y=ARRAYS OF DATA ABSCISSAA & ORDINATES
C B,C,D=ARRAYS OF SPLINE COEFFICIENTS
C
      IF(I.GE.NPTS)I=1
      IF(U.LT.X(I))GO TO 10
      IF(U.LE.X(I+1))GO TO 30
 10   I=1
      J=NPTS+1
 20   K=(I+J)/2
      IF(U.LT.X(K))J=K
      IF(U.GE.X(K))I=K
      IF(J.GT.I+1)GO TO 20
C
C EVALUATE SPLINE
C
 30   DX=U-X(I)
      SPLEVA=Y(I)+DX*(B(I)+DX*(C(I)+DX*D(I)))
      RETURN
      END
      SUBROUTINE WATER(IMON,IYR,DT,ISTEP,NSTEPS)
      COMMON/MEDIA/AWMINR,AWMOUR,WAMOUR(20),AWMINL,AWMOUL,
     $             WAMOUL,SWMINL,SWMINR,AWMINE,AWMOUE,SWMINE,WAMOUE,
     $             SAMOUL,ASMIDL,ASMIWL,SAMOUR,ASMIDR,ASMIWR,SAMOUE,
     $             ASMIDE,ASMIWE,ASMOWL,ASMODL,ASMODR,ASMOWR,
     $             ASMODE,ASMOWE,SWMOUL,SWMCUR,SWMOUE,CUMLKE,
     $             CLMLKE,CUMRIV,CLMRIV,CUMEST,CLMEST,ASMODS,ASMOWS,
     $             ASMIDS,ASMIWS,SAMOUS,CUMS,CLMS,SUMLKE,SLMLKE,CUSALK,
     $             CLSALK,LIGCUL,LIGCLL,SUMRIV,SLMRIV,CUSARV,CLSARV,
     $             LIGCUR,LIGCLR,SUMEST,SLMEST,CUSAES,CLSAES,LIGCUE,
     $             LIGCLE,SUMS,SLMS,CUSAS,CLSAS,LIGCUS,LIGCLS,CMMLKE,
     $             CMMRIV,CMMEST,CMMS,SMMLKE,SMMRIV,SMMEST,SMMS,
     $             CMSALK,CMSARV,CMSAES,CMSAS,LIGCML,LIGCMR,LIGCME,
     $             LIGCMS
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $             ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/ALPHAS/A1L,A2L,A3L,A1R,A2R,A3R,A1E,A2E,A3E,
     $              A1O,A2O,A3O
      COMMON/WPARL/WVELL(12,10),WMINL(12,10),WMTLKE,AREALK,
     $             WDEPL,WVOLL
      COMMON/WPARR/WVELR(12,10),WMINR(12,10),WMTRIV(20),
     $             NR,WWIDR,WLENR,WDEPR,WVOLR,WMTOLD,AREAR
      COMMON/WPARE/WVELE(12,10),WMINE(12,10),TIDMAX,EL,WWIDE,
     $             WLENE,WDEPE,NPTSE,AREAE
      COMMON/WPARO/WVELO(12,10),WCINO(12,10),BO,XOCEAN,NPTSO
      COMMON/WRATES/WKVL,WKPL,WKOL,WKBL,WKHL,
     $              WKVR,WKPR,WKOR,WKBR,WKHR,
     $              WKVE,WKPE,WKOE,WKBE,WKHE,
     $              WKVO,WKPO,WKOO,WKBO,WKHO
      COMMON/OUT/ACMAXL,AVAIRL,AVAIRR,AVAIRE,AWDEPL,AWDEPR,AWDEPE,
     $           ASDEPL,ASDEPR,ASDEPE,WVOLAL,WVOLAR,WVOLAE,SVOLAL,
     $           SVOLAR,SVOLAE,SWSURL,SWSURR,SWSURE,SWGRWL,SWGRWR,
     $           SWGRWE,SCONUL,SCONUR,SCONUE,SCONLL,SCONLR,SCONLE,
     $           CONL1,CONL2,CONL3,CONR1(20),CONR2(20),CONR3(20),
     $           CNCED1(11),CNCED2(11),CNCED3(11),CNCEU1(11),CNCEU2(11),
     $           CNCEU3(11),XESTY(11),CONO1(10),CONO2(10),CONO3(10),
     $           RESUSE,WASHL,WASHR,WASHE,ACMAXR,ACMAXE,ACMAXS,
     $           AVAIRS,ASDEPS,SVOLAS,SWGRWS,SCONUS,SCONLS,RESUSS,
     $           RESUSL,RESUSR,SCONML,SCONMR,SCONME,SCONMS,SWSURS,
     $           WASHS,AREA1(3)
      REAL LAKE
      DATA YES/4H YES/,NO/4H  NO/
      MON=IMON
C
C
      IF(LAKE.NE.YES)GO TO 100
C
C COMPUTE TOTAL RATE CONSTANT WKTOTL
C
      IF(MON.EQ.1.AND.ISTEP.EQ.1.AND.IYR.EQ.1)WKTOTL=
     $        WKPL+WKHL+WKOL+WKBL+WKVL
C
C WATER BODY IS A LAKE. COMPUTE TOTAL POLLUTANT SOURCE WMINLK.
C
      WMINLK=WMINL(MON,IYR)+AWMINL+SWMINL
      IF(WMINLK.EQ.0.0.AND.WMTLKE.EQ.0.0)GO TO 50
      WKDL=WVELL(MON,IYR)/SQRT(AREALK)
      WKTL=WKTOTL*A1L+WKDL
      WKTDT=-WKTL*DT
      EXWKT=EXP(WKTDT)
C
C COMPUTE MASS OF POLLUTANT IN LAKE (WMTLKE).
C
      WMTLKE=WMINLK*(1.0-EXWKT)/WKTL+WMTLKE*EXWKT
C
C CALCULATE VOLATILIZATION RATE OUT OF LAKE (WAMOUL)
C
 50   WAMOUL=WKVL*A1L*WMTLKE
      IF(ISTEP.GT.1)GO TO 75
      WVOLAL=0.0
C
C CALCULATE TOTAL MONTHLY VOLATILIZATION IN UG FROM LAKE (WVOLAL)
C
 75   WVOLAL=WVOLAL+WAMOUL*DT*1.0E+9
      IF(ISTEP.LT.NSTEPS)GO TO 100
C
C CONVERT CONCENTRATIONS TO UG/M**3 (WERE KG/M**3)
C CONL1 IS UNDISSOCIATED DISSOLVED (NEUTRAL) CONCENTRATION, CONL2 IS
C IONIC CONCENTRATION, AND CONL3 IS ADSORBED CONCENTRATION (SEDIMENT)
C
      CONL1=1.0E+9*A1L*WMTLKE/WVOLL
      CONL2=1.0E+9*A2L*WMTLKE/WVOLL
      CONL3=1.0E+9*A3L*WMTLKE/WVOLL
C
C
 100  IF(RIVER.NE.YES)GO TO 200
C
C WATER BODY IS RIVER
C
C
C COMPUTE TOTAL RATE CONSTANT WKTOTR
C
      IF(MON.EQ.1.AND.ISTEP.EQ.1.AND.IYR.EQ.1)WKTOTR=
     $         WKPR+WKHR+WKOR+WKBR+WKVR
      WKDR=WVELR(MON,IYR)/WLENR
      WKTR=WKTOTR*A1R+WKDR
      WKTDT=-WKTR*DT
      EXWKT=EXP(WKTDT)
      DO 150 I=1,NR
C
C COMPUTE TOTAL POLLUTANT SOURCE WMIN INTO REACH I
C
      WMIN=AWMINR+SWMINR/FLOAT(NR)
      IF(I.EQ.1)WMIN=WMINR(MON,IYR)+WMIN
      IF(I.GT.1)WMIN=WMIN+WKDR*WMTOLD
      IF(WMIN.EQ.0.0.AND.WMTRIV(I).EQ.0.0)GO TO 125
      WMTOLD=WMTRIV(I)
C
C CALCULATE MASS OF POLLUTANT IN REACH I (WMTRIV) AND VOLATILIZATION
C RATE FROM REACH I (WAMOUR)
C
      WMTRIV(I)=WMIN*(1.0-EXWKT)/WKTR+WMTRIV(I)*EXWKT
      WAMOUR(I)=WKVR*A1R*WMTRIV(I)
 125  IF(ISTEP.GT.1.OR.I.GT.1)GO TO 140
      WVOLAR=0.0
C
C CALCULATE TOTAL MONTHLY VOLATILIZATION IN UG FROM RIVER (WVOLAR)
C
 140  WVOLAR=WVOLAR+WAMOUR(I)*DT*1.0E+9
      IF(ISTEP.LT.NSTEPS)GO TO 150
C
C CONVERT CONCENTRATIONS TO UG/M**3 (WERE KG/M**3)
C CONR1 IS NEUTRAL FORM, CONR2 IS IONIC FORM, & CONR3 IS ADSORBED FORM
C
      CONR1(I)=1.0E+9*A1R*WMTRIV(I)/WVOLR
      CONR2(I)=1.0E+9*A2R*WMTRIV(I)/WVOLR
      CONR3(I)=1.0E+9*A3R*WMTRIV(I)/WVOLR
 150  CONTINUE
C
C
 200  IF(ESTU.NE.YES)GO TO 450
C
C WATER BODY IS ESTUARY
C
C
C COMPUTE TOTAL RATE CONSTANT WKTOTE
C
      IF(MON.EQ.1.AND.ISTEP.EQ.1.AND.IYR.EQ.1)WKTOTE=
     $        WKPE+WKHE+WKOE+WKBE+WKVE
      IF(ISTEP.GT.1)GO TO 300
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 250
      XAREAE=WWIDE*WDEPE
      WVOLE=XAREAE*WLENE
      IF(DISFLG.EQ.NO)EL=378.6359*TIDMAX**(4.0/3.0)
C
C TIDMAX IS MAXIMUM TIDAL VELOCITY IN M/S AND
C EL IS THE LONGITUDINAL DISPERSION COEFFICIENT  IN M**2/S
C
      ELTWO=2.0*EL
      WLED2=WLENE/2.0
      ESTPT=WLED2/FLOAT(NPTSE)
 250  CONTINUE
      WKTE=WKTOTE*A1E
      DISFAC=4.0*WKTE*EL
C
C WVELE IS FRESH WATER VELOCITY OF THE ESTUARY, FOLLOWING TERMS ARE
C CALCULATIONS USED IN FINAL CONCENTRATION EQUATION.
C
      ESTFAC=SQRT(WVELE(MON,IYR)*WVELE(MON,IYR)+DISFAC)
      WVELEU=(WVELE(MON,IYR)+ESTFAC)/ELTWO
      WVELED=(WVELE(MON,IYR)-ESTFAC)/ELTWO
      SOURCE=WMINE(MON,IYR)/(XAREAE*ESTFAC)
C
C SOURCE IS IN KG/M**3
C
 300  CONTINUE
C
C COMPUTE POLLUTANT SOURCE FROM AIR (AWMINE) & SOIL (SWMINE)
```

```
C
      AWMINE=AWMINE/WVOLE
      SWMINE=SWMINE/WVOLE
      WMINDK=(AWMINE+SWMINE)/WKTE
C
C WMINDK IS IN KG/M**3
C
      IF(ISTEP.LT.NSTEPS)GO TO 400
      XEST=0.0
      NPTSP1=NPTSE+1
      DO 350 I=1,NPTSP1
C
C CALCULATE CONCENTRATION IN ESTUARY AT SELECTED POINTS BOTH
C DOWNSTREAM (CONCED) & UPSTREAM (CONCEU) FROM SOURCE
C
      CONCED=WMINDK+SOURCE*EXP(WVELED*XEST)
      CONCEU=WMINDK+SOURCE*EXP(-WVELEU*XEST)
      XESTY(I)=XEST
      XEST=XEST+ESTPT
C
C COMPUTE CONCENTRATIONS IN NEUTRAL (CNCED1 & CNCEU1), IONIC (CNCED2
C & CNCEU2) AND ADSORBED FORM (CNCED3 & CNCEU3) IN UG/M**3
C
      CNCED1(I)=CONCED*A1E*1.0E+9
      CNCEU1(I)=CONCEU*A1E*1.0E+9
      CNCED2(I)=CONCED*A2E*1.0E+9
      CNCEU2(I)=CONCEU*A2E*1.0E+9
      CNCED3(I)=CONCED*A3E*1.0E+9
      CNCEU3(I)=CONCEU*A3E*1.0E+9
 350  CONTINUE
 400  CONTINUE
C
C CALCULATE POLLUTANT MASS IN ESTUARY
C
      PMASSE=WVOLE*(SOURCE*((1.0-EXP(-WVELEU*WLED2))/WVELEU+
     $       (-1.0+EXP(WVELED*WLED2))/WVELED)+
     $       WMINDK*WLENE)/WLENE
C
C CALCULATE VOLATILIZATION RATE (KG/S) TO AIR (WAMOUE)
C
      WAMOUE=WKVE*A1E*PMASSE
      IF(ISTEP.GT.1)GO TO 425
      WVOLAE=0.0
C
C COMPUTE TOTAL MONTHLY VOLATILIZATION FROM ESTUARY IN UG (WVOLAE)
C
 425  WVOLAE=WVOLAE+WAMOUE*DT*1.0E+9
C
C
 450  IF(OCEAN.NE.YES)RETURN
C
C COMPUTE TOTAL RATE CONSTANT WKTOTO
C
      IF(MON.EQ.1.AND.ISTEP.EQ.1.AND.IYR.EQ.1)WKTOTO=
     $        WKPO+WKHO+WKOO+WKBO+WKVO
      IF(ISTEP.LT.NSTEPS)RETURN
      IF(MON.GT.1.OR.IYR.GT.1)GO TO 500
C
C FACO IS 12.0*A/(B**2/3) WHERE A = .000464159 IN MKS UNITS
C
      FACO=.0055699/(BO**(2./3.))
 500  CONTINUE
      OFAC=FACO/WVELO(MON,IYR)
      WKTODV=-WKTOTO*A1O/WVELO(MON,IYR)
      OCNPT=0.0
      DO 600 I=1,NPTSO
      OCNPT=OCNPT+XOCEAN
C
C COMPUTE CONCENTRATION FOR OCEAN AT POINTS OUT FROM DIFFUSER
C
      CMAXO=WCINO(MON,IYR)*EXP(WKTODV*OCNPT)*
     $      ERF(SQRT(1.5/((1.0+2.0*OFAC*OCNPT/3.0)**3-1.0)))
C
C CALCULATE CONCENTRATIONS IN NEUTRAL (CONO1), IONIC (CONO2) AND
C ADSORBED (CONO3) FORMS IN UG/M**3.
C
      CONO1(I)=1.0E+9*A1O*CMAXO
      CONO2(I)=1.0E+9*A2O*CMAXO
 600  CONO3(I)=1.0E+9*A3O*CMAXO
      RETURN
      END
```

The following subprograms are the SESOIL routines that were modified and adopted for the TOX-SCREEN model. They are in alphabetical order.

```
      FUNCTION COMP(CONC,MWT,SK,LIGC,MWTLIG,B,THA,DPTH)
      REAL LIGC,MWT,MLC,INT,MWTLIG,MLC0
      COMP=0.0
      IF(SK .EQ. 0.0) GO TO 99
      IF(CONC.EQ.0.0)GO TO 99
      IF(LIGC.EQ.0.0)GO TO 99
C
C     SOLUTION WILL BE NEAR FULL COMPLEXATION OF EITHER LIGAND OR
C     POLLUTANT. MAKE INITIAL ESTIMATE OF COMPLEXED CONCENTRATION AND
C     DETERMINE WHICH DIRECTION TO GO.
C
C
      CP=CONC/(MWT*1.E6)
      CLIG=LIGC/(MWTLIG*1.E6)
      IF(CP .LT.  CLIG/B)GO TO 10
C
C --- LIGAND IS LIMITING REAGENT
C
      MLC0=CLIG/B
      GO TO 20
C
C --- POLLUTANT IS LIMITING REAGENT
C
   10 MLC0=CP
C
C --- TO AVOID CONVERGENCE PROBLEMS, IF CONC. OF COMPLEXED
C     POLLUTANT IS IN THE SUB PPB RANGE, SET IT TO 0. (DON'T CALC.)
C
   20 IF(MLC0*MWT*1.E6 .LT. 1.E-3)GO TO 99
C
C --- ITERATIVE SOLUTION OF EQUATION
C
C --- SET UP ITERATION PARAMETERS
C
      IFIG=0
      ISIG=0
      INT=1.E8
C
C --- FIND APPROPRIATE ITERATION INTERVAL
C
   28 IF(INT.LT.MLC0) GO TO 29
      INT=INT/10.
      GO TO 28
C
C --- USE NEGATIVE INTERVAL TO DECREASE CONCENTRATION
C
   29 INT=-1*INT
      IF(ABS(INT).LT.1.E-7)GO TO 99
      SVMLC=MLC0
      MLC=MLC0+INT
C
C --- SOLVE EQUATION SYSTEM
C     CONVERGENCE CRITERIA:BASED ON E
C
   25 SK1=MLC/((CP-MLC)*((CLIG-B*MLC)**B))
      E=SK1-SK
```

```
C
C --- TEST FOR CONVERGENCE
C
  305 AE=ABS(E)
C
C --- CONVERGENCE CRITERION 1, IS EQUATION BALANCED WITHIN 1 PERCENT
C
      IF(AE.LT. 0.01) GO TO 400
C
C --- CONVERGENCE CRITERION 2, HAS IT CROSSED THE ORIGIN(OVERSHOT)
C
      IF(E.LT.0) GO TO 402
C
C --- CONVERGENCE CRITERION 3, WILL THE NEXT STEP CAUSE A NEGATIVE
C     CONCENTRATION
C
      IF(MLC+INT .LT. 0.0)GO TO 402
C
C --- NOT CONVERGED
C
      IFIG=1
      SVMLC=MLC
      MLC=MLC+INT
      GO TO 25
C
C --- TRY SMALLER INTERVAL(CRITERIA 2 OR 3)
C
  402 IF(IFIG .EQ. 0) GO TO 410
      ISIG=ISIG+1
      IF(ISIG.EQ.6)GO TO 409
  410 INT=INT/10.
      IF(ABS(INT).LT.1.0E-8) GO TO 409
      MLC=SVMLC+INT
      GO TO 25
C
C ---STOP WHEN INTERVAL IS VERY SMALL,(I.E. CONCENTRATRATION IS
C    CALCULATED TO WITHIN NUMERICAL ACCURACY OF THE MACHINE)
C
  409 MLC=SVMLC
C
C --- FINAL CONVERGENCE OF EQUATION
C
  400 COMP=MLC*MWT*THA*DPTH*1.E6
C
C --- SET COMPLEXED MASS TO ZERO IF IN LOW RANGE
C
      IF(MLC*MWT*1.E6 .GE. 1.E-3)GO TO 99
      COMP=0.0
   99 CONTINUE
      RETURN
      END
      FUNCTION DEPTH(THA,N,IZ,RG,DO,NI)
C
C --- THIS SUBROUTINE CALCULATES THE DEPTH OF THE RAINFALL FRONT.
C
      REAL N,IZ,NI
      FLOW=(IZ+RG)
      IF(FLOW.LT.0.)FLOW=IA
      DEPTH1=FLOW/(2.*THA*N*NI)
      IF(DEPTH1 .LT. 0)DEPTH1=0.
      DEPTH=DO + DEPTH1
      RETURN
      END
      FUNCTION FGAMA(X)
C
C --- THIS SUBROUTINE HAS BEEN CODED IN FORTRAN BY P.G. EAGLESON
C          (EAGLESON,1977)
C
C
      DIMENSION B(8)
      DATA B/-0.577191165,0.98820589,-0.89705694,0.91820686,
     $-0.75670408,0.48219939,-0.19352782,0.03586834/
C
C     FOR 0<X<1, USE EIGHT POINT FORMULA FROM THE NATIONAL BUREAU
C     OF STANDARDS,'HANDBOOK OF MATHEMATICAL FUNCTIONS',
C     APPLIED MATH SERIES 55, 9-TH PRINTING,1970,PAGE 257
C
      IF(X-1.) 3,9,4
    3 XII=1./X
      X2=X
      FGAMA=XII
      GO TO 8
C --    FOR X>2, USE STERLING'S APPROXIMATION
    4 IF(X-2.) 6,9,7
    6 FGAMA=1.
      X2=X-1
      XII=1.
    8 DO 5 I=1,8
      XII=XII*X2
    5 FGAMA=FGAMA+B(I)*XII
      RETURN
    9 FGAMA=1.
      RETURN
    7 XII=1./X
      X2=XII*XII
      X3=X2*XII
      X4=X2*X2
      FGAMA=(1.0+XII/12.0+X2/288.-139./51840.*X3
     $-571./2488320.*X4)*2.506628*X**(X-0.6)*EXP(-X)
      RETURN
      END
      FUNCTION FIE(D)
C     ===============
C
C --- THIS SUBROUTINE HAS BEEN CODED IN FORTRAN BY P.G. EAGLESON
C       (EAGLESON,1977)
C
C
C     THIS FUNCTION COMPUTES THE DESORPTION COEFFICIENT BY MEANS OF A
C     LOGARITHMIC INTERPOLATION OF THE VALUES GIVEN IN THE TABLE(SEE
C     (SEE EAGLESON,1977)
C
      DIMENSION Y(6)
      DATA Y/0.18,0.11,0.077,0.056,0.044,0.034/
      IF(D.GT.7.)GO TO 11
      IF(D.LT.2.) GO TO 12
      X=D-1.
      I=IFIX(X)
      FRAC=X-FLOAT(I)
      Y1=ALOG(Y(I))
      Y2=ALOG(Y(I+1))
      FIE=EXP((Y2-Y1)*FRAC+Y1)
      RETURN
   11 FIE=0.034
      RETURN
   12 FIE=0.20
      RETURN
      END
      FUNCTION FII(D,SO,IOW)
C
C --- THIS SUBROUTINE HAS BEEN CODED IN FORTRAN BY P.G. EAGLESON
C       (EAGLESON,1977)
C
C
C     THIS FUNCTION COMPUTES THE SORPTION COEFFICIENT BY MEANS OF A
C     DOUBLE LINEAR INTERPOLATION (EAGLESON, 1977)
C
      DIMENSION DI(10,4)
      DATA DI/0.295,0.314,0.345,0.375,0.415,0.440,0.477,0.520,0.560,0.6,
     $0.234,0.254,0.280,0.310,0.345,0.382,0.428,0.478,0.537,0.6,
     $0.192,0.205,0.232,0.264,0.300,0.340,0.390,0.450,0.520,0.6,
     $0.142,0.151,0.175,0.203,0.234,0.274,0.323,0.390,0.482,0.6/
      IS=IFIX(SO*10.)
      IF(IS.GE.10) GO TO 30
      IF(D-4.) 12,11,10
   10 DD=2.
      ID1=3
      ID2=4
      X=D-4.0
      GO TO 13
   12 ID1=IFIX(D)-1
      ID2=ID1+1
      X=D-FLOAT(ID1+1)
      DD=1.0
      GO TO 13
   11 ID1=3
      ID2=3
      X=0.0
      DD=1.0
   13 IF(IS.LT.1) GO TO 20
   17 CALL LINT(DI,ID1,IS,SO,VAL1,IOW)
   14 CALL LINT(DI,ID2,IS,SO,VAL2,IOW)
   15 FII=((VAL2-VAL1)/DD)*X+VAL1
      RETURN
   20 VAL1=DI(1,ID1)
      VAL2=DI(1,ID2)
      GO TO 15
   30 FII=0.6
      RETURN
      END
      FUNCTION GAMA(A,X)
C
C --- THIS SUBROUTINE HAS BEEN CODED IN FORTRAN BY P.G. EAGLESON
C        (EAGLESON,1977)
C
C
C     THIS FUNCTION COMPUTES THE TRUNCATED GAMMA DISTRIBUTION
C     ACCORDING TO THE ALGORITHM DEVELOPED BY THE NATIONAL BUREAU OF
C     STANDARDS (HANDBOOK OF MATHEMATICAL TABLES; EAGLESON,1977)
C
C
      IF(X.EQ.0.) GO TO 13
      SUM = 1./A
      AN = 1.0
      OLD=SUM
   33 OLD=OLD*X/(A+AN)
      IF(OLD/SUM-1.E-5) 20,10,10
   10 AN=AN+1.
      SUM=SUM+OLD
      IF(AN-300.)33,33,12
   12 WRITE(IOW,100) X
  100 FORMAT(10X,'NO CONVERGENCE CAN BE OBTAINED FOR X=',E20.6)
   20 GAMA=(0.886227-EXP(A*ALOG(X)+ALOG(SUM)-X))
      RETURN
C     THE FOLLOWING STATEMENT IS A DEFINITION ONLY
   13 GAMA=0.0
      RETURN
      END
      SUBROUTINE HYDROA(L,TA,NN,S,A,REP,T,MPA,MTR,MN,MT,MH)
C
C --- THIS SUBROUTINE CALCULATES ANNUAL WATER BALANCES
C
      REAL NUT1,LOAD
      COMMON /TI/ TITLES(5,12)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /HYM/ CLIMM1(6,12,10),CLIMM2(6,12,10),CLIMM3(12,10)
      COMMON /NU/ NUT1(6)
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12)
      COMMON /HB/ HYDBAL(13,10)
      COMMON /FI/ IOR,IOW,IGE,IL0,IL1,IL2,IL3
      REAL LIGU,LIGM,LIGL
      COMMON /LEV2/PCONC(13,15,3),THM,LIGU,LIGL,LIGM
      COMMON /HYR/ THA,PA,IA,ETA,RSA,RGA,YA,GZ,SIGMA,FGAM,G,XI
      REAL L,M,C,N,K1,NU,MWA,MPA,MH,MTR,MN,MT,NN,KOC,KDE,KD,MI,MA,MTB,MB
      REAL NUT,JE,IA,KS,IAX,IAU,IAL,   K1U,K1M,K1L
C
C --- COMPILE SOIL PARAMETERS(SOIL1)
C
   12 RS = SOIL1(1)
      K1 = SOIL1(2)
      C  = SOIL1(3)
      N  = SOIL1(4)
      OC = SOIL1(5)
      CC = SOIL1(6)
      CEC= SOIL2(1)
      K1U= SOIL2(2)
      K1L= SOIL2(4)
      K1M=0.
      IF(LEVEL .GE. 3)K1M=SOIL2(3)
C
C --- COMPILE GEOMETRY DATA
C
      AR   = GEOM(1)
      Z    = GEOM(2)*100.
      DU   = GEOM(3)
      DM   = GEOM(4)
C
C --- CALCULATE AVERAGE PERMEABILITY (IF NECESSARY)
C
      IF(K1 .NE. 0.0 )GO TO 15
      DL = Z -(DU+DM)
      K1=(DU+DL)/((DU/K1U)+(DL/K1L))
      IF(LEVEL .GE.3) K1=(DU+DM+DL)/((DU/K1U)+(DM/K1M)+(DL/K1L))
C
C --- SET CONSTANTS (LATENT HEAT OF VAP.;WATER DENSITY)
C
   15 HLE=597.
      RW=1.0
C
C --- COMPUTE BASIC PARAMETERS  (STEPS 1-9)
C
      MI=MH/MTR
      ALFA=1./MI
      MTB=(MT/MN)-MTR
      BETA=1./MTB
      ETHA=1./MH
      DELTA=1./MTR
      M =2./(C-3.)
      D =(C+1.)/2.
      FC = 10.**(0.66+(0.55/M)+(0.14/M**2.))
C
C --- COMPUTE WATER CONSTANTS
C         SUT=SATURATION
C         NU=VISCOSITY
C         GAMSW=SPECIFIC WEIGHT OF WATER
C
      CALL WATCN(TA,SUT,NU,GAMSW)
C
C---  COMPUTE WAT.BUDGET PARAMETERS  (STEPS 10-21)
C
      SG=SUT/GAMSW
      PSI1= SG*SQRT(N/(K1*FC))
      BK1 = K1*GAMSW*86400./NU
      B = 1.+((3./2.)/(M*C-1.))
      W = B*BK1*((PSI1/Z)**(M*C))
      IF(REP.GT.0.) GO TO 20
      QI = 0.358-0.004*(L-25.)
      QB = (1.-0.8*NN)*(0.245-0.145*(10.**(-10.))*(TA**4.))
      H = QB/(0.25+(1./(1.-S)))
      DB=0.42+0.013*TA
      EP = 60.*24.*(QI*(1.-A)-QB+H)/(RW*HLE/DB)
      GO TO 21
   20 QI=0.
      QB=0.0
      H=0.0
      DB=0.0
      EP=REP
   21 EEPA=MT*EP
C ********************************
      IF(W.LT.EP) GO TO 22
            W=0.99*EP
            WRITE(IOW,444)
  444 FORMAT('1',15(/),10X,'*************WARNING*************',///,
     110X,'USE OF SMALL SOIL PERMEABILITY AND/OR GROUNDWATER DEPTH',/,
     210X,'HAVE CAUSED THE CALCULATED CAPILLARY RISE VELOCITY(W) TO',/,
     310X,'BE GREATER THAN THE POTENTIAL EVAPOTRANSPIRATION RATE(EP),',
     4/,10X,'A VIOLATION TO THE MODEL ASSUMPTION.  TO ENSURE THE CON-',
     5/,10X,'TINUITY OF THE MODEL EXECUTION, W IS RESET TO W=0.99(EP).'
     6/,10X,'MODEL OUTPUT MAY GIVE ONLY APPROXIMATE SOLUTIONS AND',/,
     710X,'MUST BE INTERPRETED WITH CAUTION.')
C ********************************
22    FIED=FIE(D)
C
C --- START ITERATIVE PROCEDURE TO SOLVE WATER BALANCE
C
      SO=.038059*(1.0/K1**0.0466573)*C**0.757928
      IFLAG=1
      ISW=0
```

```
C
C --- COMPUTE FUNCTIONS (STEPS 22-25)
C
  800 E = ((2.*BETA*N*BK1*PSI1*FIED)/(3.1415927*M*((ABS(EP-W))**2.)))
     $*(SO**(D+2.))
      IF(E.GT.10.)GO TO 10
      GAM=GAMA(1.5,E)
      JE = 1.-(1.+1.414114*E)*EXP(-E)+SQRT(2.*E)*GAM
      GO TO 101
   10 JE =1.0
  101 CONTINUE
C
C --- COMPUTE MATRIX POTENTIAL COEFFICIENTS (STEPS 26-30)
C
      FIID = FII(D,SO,IOW)
      SIGMA=((5.*N*(ETHA**2.)*BK1*PSI1*((1.-SO)**2.)*FIID)/(6.*3.1415927
     $*DELTA*M))**(1./3.)
      FGAM = FGAMA(SIGMA+1.)
      G = 0.5*ALFA*BK1*(1.+SO**C)-ALFA*W
      XI = EXP(-2.*SIGMA)*FGAM/(SIGMA**SIGMA)
C
C --- COMPUTE WATER BALANCE COMPONENTS (STEPS 31-36)
C
      IF(REP .GT. 0.0)ETA=EEPA
      IF(REP .EQ. 0.0)ETA=EEPA*JE
      PA = (ETA+(MT*BK1*(SO**C))-T*W)/(1.-EXP(-G)*XI)
      IA = PA*(1.-EXP(-G)*XI)
      RSA= PA*(EXP(-G)*XI)
      RGA=MT*BK1*(SO**C)-T*W
      YA = RSA+RGA
C
C --- TEST FOR CONVERGENCE
C
C --- AGREEMENT TO WITHIN .1%
C
      GZ = PA/MPA
      IF(GZ.GE.1.01.AND.IFLAG.EQ.1)ISW=1
      IFLAG=2
      IF(ISW.EQ.1)GO TO 25
      IF(GZ.GT.0.999) GO TO 70
C
C --- NOT CONVERGED
C
 23   CONTINUE
      ISW=0
      DSO=0.001
      SO=SO+DSO
      IF(SO.GT.1.)GO TO 999
      GO TO 800
 25   IF(GZ.LT..99)GO TO 23
      IF(GZ.LT.1.01)GO TO 70
      DSO=0.001
      SO=SO-DSO
      GO TO 800
C
C --- CALCULATE ACTUAL SOIL MOISTURE CONTENT THA=SO*N
```

```
C
   70 THA=SO*N
C
C --- RETURN TO LEVEL ROUTINE
C
      RETURN
  999 WRITE(9,903)
  903 FORMAT('SO OUT OF BOUNDS')
      STOP
      END
      SUBROUTINE HYDROM(IYR,IMO)
C
C     THIS SUBROUTINE ESTIMATES THE MONTHLY HYDROLOGIC CYCLE COMPONENTS
C
      REAL NUT1,LOAD
      COMMON /TI/ TITLES(5,12)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /HYM/ CLIMM1(6,12,10),CLIMM2(6,12,10),CLIMM3(12,10)
      COMMON /NU/ NUT1(6)
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12)
      COMMON /HB/ HYDBAL(13,10)
      COMMON /FI/ IOR,IOW,IGE,IL0,IL1,IL2,IL3
      REAL LIGU,LIGM,LIGL
      COMMON /LEV2/PCONC(13,15,3),THM,LIGU,LIGL,LIGM
      COMMON /HYR/ THA1,PA1,IA1,ETA1,RSA1,RGA1,YA1,GE1,SIGMA1,FGAM1,G1,
     *XI1
      DIMENSION HYDRO(6)
      REAL L,M,C,N,K1,NU,MWA,MPA,MH,MTR,MN,MT,NN,KOC,KDE,KD,MI,MA,MTB
      REAL MB,NUT,JE,IA,KS,IAX,IAU,IAL,K1U,K1M,K1L
      REAL NNSUM,MPASUM,MTRSUM,MNSUM,MTSUM,MHSUM,IA1
C
C --- INITIALIZE HYDBAL ARRAY AND SUM VARIABLES
C
      IF(IMO.GT.1)GO TO 100
      DO 1 IJ=1,13
      DO 1 IK=1,10
    1 HYDBAL(IJ,IK)=0.0
      TASUM = 0.0
      NNSUM = 0.0
      SSUM = 0.0
      ASUM  =0.0
      REPSUM = 0.0
      MPASUM= 0.0
      MTRSUM = 0.0
      MNSUM = 0.0
      MTSUM = 0.0
C
C --- COMPILATION OF INITIAL CLIMATIC PARAMETERS (FOR FIRST YEAR ONLY)
C     BASED UPON THE LONG TERM ANNUAL AVERAGES OF THIS YEAR
C
      L  = CLIMM1(1,1,IYR)
      IF(IYR.NE.1.OR.IMO.GT.1)GO TO 100
      DO 5  IMO=1,12
      TASUM =TASUM + CLIMM1(2,IMO,IYR)
      NNSUM =NNSUM +  CLIMM1(3,IMO,IYR)
      SSUM = SSUM + CLIMM1(4,IMO,IYR)
      ASUM  =ASUM + CLIMM1(5,IMO,IYR)
      REPSUM = REPSUM + CLIMM1(6,IMO,IYR)
      MPASUM= MPASUM + CLIMM2(1,IMO,IYR)
      MTRSUM = MTRSUM + CLIMM2(2,IMO,IYR)
      MNSUM =MNSUM + CLIMM2(3,IMO,IYR)
      MTSUM =MTSUM +  CLIMM2(4,IMO,IYR)
C
    5 CONTINUE
```

```
      IMO=1
      TASUM=TASUM/12.
      NNSUM=NNSUM/12.
      SSUM=SSUM/12.
      ASUM=ASUM/12.
      REPSUM=REPSUM/12.
      MTRSUM=MTRSUM/12.
      MHSUM=MPASUM/MNSUM
      T=365.
C
C --- COMPILATION OF SOIL PARAMETERS (STORED IN ARRAY SOIL1)
C
      RS = SOIL1(1)
      K1 = SOIL1(2)
      C  = SOIL1(3)
      N  = SOIL1(4)
      OC = SOIL1(5)
      CC = SOIL1(6)
      K1U= SOIL2(2)
      K1L= SOIL2(4)
      IF(LEVEL .GE. 3)K1M= SOIL2(3)
C
C --- COMPILATION OF GEOMETRIC PARAMETERS
C
      AR  = GEOM(1)
      Z   = GEOM(2)*100.
      DU  = GEOM(3)
      DM  = GEOM(4)
C
C --- CALCULATE AVERAGE PERMEABILITY (IF NECESSARY)
C
      IF(K1 .NE. 0.0 )GO TO 14
      DL = Z -(DU+DM)
      K1=(DU+DL)/((DU/K1U)+(DL/K1L))
      IF(LEVEL .GE.3) K1=(DU+DM+DL)/((DU/K1U)+(DM/K1M)+(DL/K1L))
C
C --- FOR FIRST YEAR ONLY , RUN HYDROA TO GET AN ESTIMATE FOR INITIAL
C --- MOISTURE CONTENT AND OTHER PARAMETERS
C
   14 CALL HYDROA(L,TASUM,NNSUM,SSUM,ASUM,REPSUM,T,MPASUM,MTRSUM,
     *MNSUM,MTSUM,MHSUM)
C
C --- ESTIMATION OF MONTHLY HYDROLOGIC CYCLE COMPONENTS
C --- RUN FOR 12 MONTHS
C
  100 CONTINUE
C
C --- COMPILATION OF CLIMATIC PARAMETERS  (LEVELS 2 & 3)
C
      L  = CLIMM1(1,1,IYR)
      TA = CLIMM1(2,IMO,IYR)
      NN = CLIMM1(3,IMO,IYR)
      S  = CLIMM1(4,IMO,IYR)
      A  = CLIMM1(5,IMO,IYR)
      REP= CLIMM1(6,IMO,IYR)
C
```

```
C --- COMPILATION OF TIME & RAINFALL PARAMETERS  (LEVELS 2 & 3)
C
      T  = 365.
      MPA= CLIMM2(1,IMO,IYR)*12.
      MTR= CLIMM2(2,IMO,IYR)
      MN = CLIMM2(3,IMO,IYR)*12.
      MT = CLIMM2(4,IMO,IYR)*12.
C
C --- CONSTANT VALUES (LATENT HEAT OF VAP.;WATER DENSITY)
C
      HLE=597.
      RW=1.0
C
C --- IF MONTHLY RAINFALL IS NOT 0.0, PROCEED AS USUAL
C     OTHERWISE SEE BELOW STATEMENT FOR ZERO RAINFALL CONSTRAINT
C
      IF(MPA.GT.0.0)GO TO 15
C
C --- FOR MPA=0.0  ASSUME BASIC CLIMATIC PARAMETERS  (STEPS 1-6)
C     HAVING A NEGLIGIBLE VALUE. THIS CONSTRAINT IS NOT USED
C
C     MPA=0.1
C     MTR = 0.20
C     MN = 1.0
C     MT = 0.5
C
C --- ALTERNATIVE CONSTRAINTS FOR MPA=0.0
C
      MPA= 0.0
      MTR= 0.0
      MN = 0.0
      MT = 0.0
      MH = 0.0
      MI = 0.0
      MTB= 365./12.
      BETA=12./365.
      GO TO 16
C
C --- ESTIMATE BASIC SYNTHETIC PARAMETERS(FOR MPA NOT = 0.) (STEPS 1-9)
C
   15 MH=MPA/MN
      MI=MH/MTR
      ALFA=1./MI
      MTB=(MT/MN)-MTR
      BETA=1./MTB
      ETHA=1./MH
      DELTA=1./MTR
C
   16 M =2./(C-3.)
      D =(C+1.)/2.
      FC = 10.**(0.66+(0.55/M)+(0.14/M**2.))
C
C --- COMPUTE WATER CONSTANTS
C          SUT=SATURATION
C          NU=VISCOSITY
C          GAMSW=SPECIFIC WEIGHT OF WATER
```

```
      CALL WATCN(TA,SUT,NU,GAMSW)
C
C---  COMPUTE WATER BUDGET PARAMETERS  (STEPS 10-21)
C
      SG=SUT/GAMSW
      PSI1= SG*SQRT(N/(K1*FC))
      BK1 = K1*GAMSW*86400./NU
      B = 1.+((3./2.)/(M*C-1.))
      W = B*BK1*((PSI1/Z)**(M*C))
      IF(REP.GT.0.) GO TO 20
      QI = 0.358-0.004*(L-25.)
      IF(TA.GE.0.0) GO TO 411
         QB = (1.-0.8*NN)*(0.245-0.145*(10.**(-10.))*(0.0))
         GO TO 412
411   QB = (1.-0.8*NN)*(0.245-0.145*(10.**(-10.))*(TA**4.))
412   H = QB/(0.25+(1./(1.-S)))
      DB=0.42+0.013*TA
      EP = 60.*24.*(QI*(1.-A)-QB+H)/(RW*HLE/DB)
      GO TO 21
   20 QI=0.
      QB=0.0
      H=0.0
      DB=0.0
      EP=REP
   21 EEPA=MT*EP
C *******************************
      IF(W.GE.EP) W=0.99*EP
C *******************************
      FIED=FIE(D)
C
C --- START ITERATIVE PROCEDURE TO OBTAIN SOLUTION OF HYD.BALANCE EQUAT.
C
      SO=THA1/N
      ISW=0
      IFLAG=1
C
C --- COMPUTE FUNCTIONS (STEPS 22-25)
C
  800 E = ((2.*BETA*N*BK1*PSI1*FIED)/(3.1415927*M*((ABS(EP-W))**2.)))
     $*(SO**(D+2.))
      IF(E.GT.10.)GO TO 10
      GAM=GAMA(1.5,E)
      JE = 1.-(1.+1.414114*E)*EXP(-E)+SQRT(2.*E)*GAM
      GO TO 101
   10 JE =1.0
  101 CONTINUE
C
C --- COMPUTE MATRIX POTENTIAL COEFFICIENTS (STEPS 26-30)
C
      FIID = FII(D,SO,IOW)
C
C --- IF MPA NOT = 0, PROCEED AS USUAL
C
      IF(MPA .GT. 0) GO TO 17
C
C --- IF MPA = 0, SET BELOW SOIL-MOISTURE INSENSITIVE PARAMETERS
```

```
C       TO PREVIOUS MONTHLY VALUES. THIS SECTION IS OPERATIONAL
C
      SIGMA = SIGMA1
      FGAM = FGAM1
      G = G1
      XI = XI1
      GO TO 18
C
C --- FOR MPA NOT = 0, CALCULATE PARAMETERS
C
   17 SIGMA=((5.*N*(ETHA**2.)*BK1*PSI1*((1.-SO)**2.)*FIID)/(6.*3.1415927
     $*DELTA*M))**(1./3.)
      IF(SIGMA.GT.25.0)SIGMA=25.0
      FGAM = FGAMA(SIGMA+1.)
      G = 0.5*ALFA*BK1*(1.+SO**C)-ALFA*W
      XI = EXP(-2.*SIGMA)*FGAM/(SIGMA**SIGMA)
C
   18 CONTINUE
C
C
C --- ESTIMATION OF HYDROLOGIC CYCLE COMPONENTS (STEPS 31-36)
C
      SO1=THA1/N
      IF(REP .GT. 0.0)ETA=EEPA
      IF(REP .EQ. 0.0)ETA=EEPA*JE
      PA=(ETA+(MT*BK1*(SO**C))-(T*W)+(N*E*(SO-SO1)))/(1.-EXP(-G)*XI)
      IA = PA*(1.-EXP(-G)*XI)
      RSA= PA*(EXP(-G)*XI)
      RGA= MT*BK1*(SO**C)-T*W
      YA = RSA+RGA
C
C --- CONVERGENCE CRITERION FOR MPA=0.0
C
      IF(MPA.GT.0.0) GO TO 22
      IF(PA.GT.0.0) GO TO 70
      GO TO 23
C
C --- TEST FOR CONVERGENCE
C --- TO WITHIN .1%
C
   22 GE = PA/MPA
      IF(GE.GE.1.01.AND.IFLAG.EQ.1)ISW=1
      IFLAG=2
      IF(ISW.EQ.1)GO TO 25
      IF(GE.GT.0.99) GO TO 70
C
   23 CONTINUE
C
C
C --- CONVERGENCE NOT ACHIEVED, REPEAT SO LOOP
C
      ISW=0
      DSO=0.001
      SO=SO+DSO
      GO TO 800
   25 IF(GE.LT.0.99)GO TO 23
```

```
      IF(GZ.LT.1.01)GO TO 70
      DSO=0.001
      SO=SO-DSO
      GO TO 800
C
C --- ESTIMATE  ACTUAL SOIL MOISTURE CONTENT THA=SO*N
C
   70 THA=SO*N
      THA1=THA
      PA1=PA
      IA1=IA
      ETA1=ETA
      RSA1=RSA
      YA1=YA
      GZ1=GZ
      SIGMA1=SIGMA
      FGAM1=FGAM
      G1=G
      XI1=X1
C
C --- STORE MONTHLY SIMULATION RESULTS IN HYDBAL ARRAY
C
      HYDBAL(IMO,1)=THA
      HYDBAL(IMO,2)=PA/12.
      HYDBAL(IMO,3)=IA/12.
      HYDBAL(IMO,4)=ETA/12.
      HYDBAL(IMO,5)=RSA/12.
      HYDBAL(IMO,6)=RGA/12.
      HYDBAL(IMO,7)=YA/12.
      HYDBAL(IMO,8)=GZ
      HYDBAL(IMO,9)=CLIMM2(1,IMO,IYR)
  500 CONTINUE
C
C --- THIS YEAR'S SIMULATION ACCOMPLISHED RETURN TO LEVEL ROUTINE
C
      RETURN
      END
      SUBROUTINE LEVEL3
C     =================
C
C     THIS SUBROUTINE ESTIMATES THE MONTHLY HYDROLOGIC CYCLES AND
C     CONSEQUENTLY GIVES A FATE ASSESSMENT FOR THE COMPOUND. THIS
C     LEVEL MODELS 3 SOIL LAYERS, WITH A MONTHLY TIME STEP.
C
      REAL NUT1,LOAD
      COMMON /TI/ TITLES(5,12)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /HYM/ CLIMM1(6,12,10),CLIMM2(6,12,10),CLIMM3(12,10)
      COMMON /NU/ NUT1(6)
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12)
      COMMON /HB/ HYDBAL(13,10)
      COMMON /FI/ IOR,IOW,IGE,IL0,IL1,IL2,IL3
      REAL LIGU,LIGM,LIGL,IA
      COMMON /LEV2/PCONC(13,15,3),THM,LIGU,LIGL,LIGM
      COMMON /HYR/ THA,PA,IA,ETA,RSA,RGA,YA,GE,SIGMA,FGAM,G,XI
      COMMON/SPARE/ARE,AREASE
      COMMON/SPARR/ARR,AREASR
      COMMON/SPARL/ARL,AREASL,XSOIL
      COMMON/SPARS/ARS,AREAS,XLENS
      COMMON/MEDIA/AWMINR,AWMOUR,WAMOUR(20),AWMINL,AWMOUL,
     $             WAMOUL,SWMINL,SWMINR,AWMINE,AWMOUE,SWMINE,WAMOUE,
     $             SAMOUL,ASMIDL,ASMIWL,SAMOUR,ASMIDR,ASMIWR,SAMOUE,
     $             ASMIDE,ASMIWE,ASMOWL,ASMODL,ASMODR,ASMOWR,
     $             ASMODE,ASMOWE,SWMOUL,SWMOUR,SWMOUE,CUMLKE,
     $             CLMLKE,CUMRIV,CLMRIV,CUMEST,CLMEST,ASMODS,ASMOWS,
     $             ASMIDS,ASMIWS,SAMOUS,CUMS,CLMS,SUMLKE,SLMLKE,CUSALK,
     $             CLSALK,LIGCUL,LIGCLL,SUMRIV,SLMRIV,CUSARV,CLSARV,
     $             LIGCUR,LIGCLR,SUMEST,SLMEST,CUSAES,CLSAES,LIGCUE,
     $             LIGCLE,SUMS,SLMS,CUSAS,CLSAS,LIGCUS,LIGCLS,CMMLKE,
     $             CMMRIV,CMMEST,CMMS,SMMLKE,SMMRIV,SMMEST,SMMS,
     $             CMSALK,CMSARV,CMSAES,CMSAS,LIGCML,LIGCMR,LIGCME,
     $             LIGCMS
      COMMON/SDPARO/SEDCO(12,10),CONSDO
      COMMON/SDPARE/SEDCE(12,10),CONSDE
      COMMON/SDPARL/SEDCL(12,10),DIASDT,DENSDT,DENWT,SLOPET,WDEPT,CONSDL
      COMMON/SDPARR/SEDCR(12,10),DIASDR,DENSDR,DENWR,SLOPER,CONSDR
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $             ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      REAL NO,LAKE
      DIMENSION AMO(12),HYDOUT(12)
      DATA AMO/' OCT',' NOV',' DEC',' JAN',' FEB',' MAR',
     *' APR',' MAY',' JUN',' JUL',' AUG',' SEP'/
      DATA NO/4H  NO/,YES/4H YES/
C
C --- INITIALIZE ARRAYS
C
      DO 1 IWATER=1,3
      DO 1 I=1,12
      DO 1 J=1,15
      PCONC(I,J,IWATER)=0.0
    1 CONTINUE
```

```
C
C --- PRINT TITLES AND INPUT VARIABLES
C
      WRITE(IOW,703)
  703 FORMAT('1',/,1X,77('*'),/)
      WRITE(IOW,700)JRUN
  700 FORMAT(/,/,1X,'RUN :',I3,T25,'****** LEVEL3 SESOIL MODEL ',
     *'OPERATION ******',/,T26,'MONTHLY SITE SPECIFIC SIMULATION(3 LAY',
     *'ERS)',/,/)
      WRITE(IOW,901)
  901 FORMAT(/,/,5X, 99('*'),/,5X,'*****',T100,'*****',/,
     *5X,'***** SESOIL-82:   SEASONAL CYCLES OF WATER, SEDIMENT, ',
     1'AND POLLUTANTS IN SOIL ENVIRONMENTS',T100,'*****',/,
     2 5X,'*****',T100,'*****')
      WRITE (IOW,902)
  902 FORMAT(5X,'***** DEVELOPERS:  M. BONAZOUNTAS,ARTHUR D. LITTLE INC.
     1  ,(617)864-5770,X5871',T100,'*****')
      WRITE(IOW,903)
  903 FORMAT(5X,'*****                J. WAGNER      ,ARTHUR D. LITTLE INC.
     1  ,(617)864-5770,X2585',T100,'*****',/,
     2 5X,'*****',T100,'*****')
      WRITE(IOW,905)
  905 FORMAT(5X,'***** VERSION:      JULY 1982',T100,'*****',/,
     * 5X,'*****',T100,'*****',/,5X,'*****',T100,'*****',/,
     *5X,99('*'),/,/,23X,'INDEX')
      WRITE(IOW,702)JRE,(TITLES(1,IQ),IQ=1,12),
     *JSO,(TITLES(2,IR),IR=1,12),
     *JCH,(TITLES(3,IS),IS=1,12),
     *JAPPL,(TITLES(5,IT),IT=1,12)
  702 FORMAT(10X,'REGION     : (',I5,')',T35,12A4,/
     *10X,'SOIL TYPE : (',I5,')',T35,12A4,/,
     *10X,'COMPOUND  : (',I5,')',T35,12A4,/,
     *10X,'APPL. AREA: (',I5,')',T35,12A4)
      WRITE(IOW,705)(GEOM(IQ),IQ=1,4),GEOM(14)
  705 FORMAT(/,/,10X,'GENERAL INPUT PARAMETERS',/,10X,24('='),4(/),6X,
     *'-- APPLICATION PARAMETERS --',/,/,1X,'AREA(SQ.CM): ',G7.2,/,1X,
     *'DEPTH TO GRW(M): ',G7.2,/,1X,'UPPER SOIL ZONE DEPTH(CM): ',
     *G7.2,/,1X,'MIDDLE SOIL ZONE DEPTH(CM): ',G7.2,/,1X,
     *'FREUNDLICH EXPONENT(-): ',G7.2)
      WRITE(IOW,711)GEOM(15),GEOM(16),GEOM(17)
  711 FORMAT(1X,'PH UPPER ZONE(-): ',G7.2,/,
     *1X,'PH RATIO MIDDLE:UPPER ZONE(-): ',G7.2,/
     *1X,'PH RATIO LOWER:UPPER ZONE(-): ',G7.2)
      WRITE(IOW,712)GEOM(6),GEOM(9),GEOM(7),GEOM(10),GEOM(8),GEOM(11)
  712 FORMAT(1X,'DEGRADATION RATIO MIDDLE:UPPER ZONE(-): ',
     *G7.2,/,1X,'DEGRADATION RATIO LOWER:UPPER ZONE(-): ',G7.2
     *,/,1X,'ORGANIC CARBON CONTENT RATIO MIDDLE:UPPER ZONE(-): ',
     *G7.2,/,1X,'ORGANIC CARBON CONTENT RATIO LOWER:UPPER ZONE(-):
     *',G7.2,/,1X,'CLAY CONTENT RATIO MIDDLE:UPPER ZONE(-): ',G7.2,
     */,1X,'CLAY CONTENT RATIO LOWER:UPPER ZONE(-): ',G7.2)
      WRITE(IOW,725)GEOM(18),GEOM(19)
  725 FORMAT(1X,'CATION EXCHANGE CAPACITY RATIO MIDDLE:LOWER ZONE(-): ',
     *G7.2,/,1X,'CATION EXCHANGE CAPACITY RATIO LOWER:UPPER ZONE(-): ',
     *G7.2)
      WRITE(IOW,708)(CHEM1(IQ),IQ=1,6)
  708 FORMAT('1',5(/),6X,'-- CHEMICAL PARAMETERS --',/,/,1X,
     *'SOLUBILITY(UG/ML): ',G7.2,/,1X,'ADSORP. COEF.(KOC): ',G7.2,/,1X,
     *'DIF. COEF. IN AIR(SQ.CM/SEC): ',G7.2,/,1X,
     *'DEGRADATION RATE(/DAY): ',G7.2,/,1X,'HENRYS CON.(CU.M-ATM/MOLE):
     *',G7.2,/,1X,'ADSORP. COEF. ON SOIL(K): ',G7.2)
      WRITE(IOW,709)(CHEM1(IQ),IQ=7,11)
  709 FORMAT(1X,
     *'MOLECULAR  WT.(G/MOL): ',G7.2,/,1X,'VALENCE(-): ',G7.2,/,1X,
     *'NEUTRAL HYDROLYSIS CONSTANT(/DAY): ',G7.2,/,1X,
     *'BASE HYDROLYSIS CONSTANT(L/MOL-DAY): ',G7.2,/,1X,
     *'ACID HYDROLYSIS CONSTANT(L/MOL-DAY): ',G7.2)
      WRITE(IOW,713)(CHEM1(IQ),IQ=13,15)
  713 FORMAT(1X,
     *'LIGAND-POLLUTANT STABILITY CONST.(-): ',G7.2,/,1X,
     *'NO. MOLES LIGAND/MOLE POLLUTANT(-): ',G7.2,/,1X,
     *'LIGAND MOLECULAR WEIGHT(G/MOL): ',G7.2)
      WRITE(IOW,710)(SOIL1(IQ),IQ=1,6)
  710 FORMAT(/,/,6X,'-- SOIL PARAMETERS --',/,/,1X,
     *'DENSITY(G/CU.CM): ',G7.2,/,1X,'INT. PERMEABILITY(SQ.CM): ',
     *G7.2,/,1X,'DISCONNECTEDNESS INDEX(-): ',G7.2,/,1X,'POROSITY(-): ',
     *G7.2,/,1X,'ORGANIC CARBON CONTENT(%): ',G7.2,/,1X,
     *'CLAY CARBON CONTENT(%): ',G7.2)
      WRITE(IOW,714)(SOIL2(IQ),IQ=1,5)
  714 FORMAT(1X,
     *'CATION EXCHANGE CAP.  (MILLI EQ./100G DRY SOIL): ',G7.2,/,1X,
     *'INTRINSIC PERMEABILITY-UPPER ZONE(SQ.CM): ',G7.2,/,1X,
     *'INTRINSIC PERMEABILITY-MIDDLE ZONE(SQ.CM): ',G7.2,/,1X,
     *'INTRINSIC PERMEABILITY-LOWER ZONE(SQ.CM): ',G7.2,/,1X,
     *'DUST LOADING FACTOR (UG(SOIL)/M**3): ',G7.2)
      IF(JYRS .LT. 1)JYRS=1
C
C --- RUN FOR JYRS
C
C --- INITIALIZE AREA OF DIRECT APPLICATION FOR EACH WATER BODY CASE
C --- AND AREA OF SOIL NEXT TO EACH WATER BODY COVERED BY PLUME.
C
      ARE=GEOM(1)
      AREASE=ARE*.0001
      ARR=GEOM(1)
      AREASR=ARR*.0001
      ARL=GEOM(1)
      AREASL=ARL*.0001
      ARS=GEOM(1)
      AREAS=ARS*.0001
C
C --- TIME STEP IS 3 DAYS, NSTEPS IS NUMBER OF STEPS PER MONTH
C
      DT=3.0*24.0*3600.0
      NSTEPS=10
      DO 720 I=1,JYRS
C
C --- IF NOT FIRST YEAR,READ APPLICATION DATA FROM FILE: L3 DATA
C
      IF(I.EQ.1) GO TO 718
      READ(IL3,906)(RUNM1(1,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(2,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(3,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(4,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(5,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(6,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(7,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(1,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(2,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(3,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(4,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(5,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(6,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(7,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(8,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(9,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(10,IQ),IQ=1,12)
  906 FORMAT(8X,12F6.2)
 9061 FORMAT(8X,12F6.2)
C
C --- PRINT ANNUAL INPUT DATA (MONTHLY PRECIPITAION,CLIMATIC
C       PARAMETERS, AND APPLICATION DATA)
C
  718 WRITE(IOW,722)I,(AMO(IQ),IQ=1,12)
  722 FORMAT('1',1(/),1X,131('-'),/,/,
     *3(/),25X,'YEAR-',I2,2X,'MONTHLY INPUT PARAMETERS',/,25X,7('='),
     *2X,24('='),/,/,/,
     *18X,12(2X,A4,3X),/,/)
      WRITE(IOW,706)((CLIMM1(IR,IQ,I),IQ=1,12),IR=1,6)
      WRITE(IOW,719)((CLIMM2(IR,IQ,I),IQ=1,12),IR=1,4)
  706 FORMAT(/,/,6X,'-- CLIMATIC PARAMETERS --',/,/,1X,
     *'LATITUDE(DEG) ',T20,12G9.3,/,1X,'TEMP.(DEG C) ',T20,12G9.3,/,
     *1X,'CLOUD CVR(FRAC.) ',T20,12G9.3,/,1X,'REL. HUMID.(FRAC.) ',
     *T20,12G9.3,/,1X,'ALBEDO(-) ',T20,12G9.3,/,1X,
     *'EVAPOT.(CM/DAY) ',T20,12G9.3)
  719 FORMAT(/,1X,'PRECIP.(CM) ',T20,12G9.3,/,1X,
     *'M.TIME RAIN(DAYS) ',T20,12G9.3,/,1X,
     *'M. STORM NO.(-) ',T20,12G9.3,/,1X,
     *'M. SEASON(DAYS) ',T20,12G9.3)
      WRITE(IOW,721)(RUNM1(1,IQ),IQ=1,12),(RUNM1(2,IQ),IQ=1,12),
     *(RUNM1(3,IQ),IQ=1,12),(RUNM1(4,IQ),IQ=1,12),
     *(RUNM1(5,IQ),IQ=1,12)
  721 FORMAT(5(/),6X,'-- RUN DATA-SET 1 --',/,/,1X,'MOIS. CONC-UP.'
     *,'(UG/ML)',T24,12G9.3,/,1X,'MOIS. CONC-MI.(UG/ML)',T24,12G9.3
     *,/,1X,'MOIS. CONC-LO.(UG/ML)',T24,12G9.3
     *,/,1X,'POL. INP-U(UG/SQ.CM)',T24,12G9.3,
     */,1X,'POL. INP-M(UG/SQ.CM)',T24,12G9.3)
      WRITE(IOW,716)(RUNM1(6,IQ),IQ=1,12),(RUNM1(7,IQ),IQ=1,12)
  716 FORMAT(1X,
     *'POL. INP-L(UG/SQ.CM)',T24,12G9.3,
     */,1X,'SUR. RUNOFF(1=Y,0=N)',T24,12G9.3)
      WRITE(IOW,717)(RUNM2(1,IQ),IQ=1,12),(RUNM2(2,IQ),IQ=1,12),
     *(RUNM2(3,IQ),IQ=1,12),(RUNM2(4,IQ),IQ=1,12),
     *(RUNM2(5,IQ),IQ=1,12)
  717 FORMAT(/,/,6X,'-- RUN DATA-SET 2 --',/,/,1X,'CONC. IN RAIN(UG'
     *,'/ML)',T24,12G9.3,/,1X,'TRNSFORMED-U(UG/SQ.CM)',T24,12G9.3,
     */,1X,'TRNSFORMED-M(UG/SQ.CM)',T24,12G9.3,
     */,1X,'TRNSFORMED-L(UG/SQ.CM)',T24,12G9.3,
     */,1X,'SINKS-U(UG/SQ.CM)',T24,12G9.3)
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      WRITE(IOW,715)(RUNM2(6,IQ),IQ=1,12),(RUNM2(7,IQ),IQ=1,12),
     *(RUNM2(8,IQ),IQ=1,12),(RUNM2(9,IQ),IQ=1,12),
     *(RUNM2(10,IQ),IQ=1,12)
  715 FORMAT(1X,'SINKS-M(UG/SQ.CM)',T24,12G9.3,/,1X,
     *'SINKS-L(UG/SQ.CM)',T24,12G9.3,/,1X,
     *'LIG.INPUT-U(UG/SQ.CM)',T24,12G9.3,/,1X,
     *'LIG.INPUT-M(UG/SQ.CM)',T24,12G9.3,/,1X,
     *'LIG.INPUT-L(UG/SQ.CM)',T24,12G9.3)
C
C --- RUN FOR HYDRO CYCLE FOR 1 YEAR
C
      DO 720 IMO=1,12
      CALL HYDROM(I,IMO)
C
C --- FIND SEDIMENT CONCENTRATION FOR EACH WATER BODY
C
      IF(SEDLKE.EQ.YES.AND.LAKE.EQ.YES) CONSDL=SEDCL(IMO,I)
      IF(SEDRIV.EQ.YES.AND.RIVER.EQ.YES) CONSDR=SEDCR(IMO,I)
      IF(SEDLKE.EQ.NO.OR.SEDRIV.EQ.NO) CALL SEDCON(IMO,I)
      IF(ESTU.EQ.YES) CONSDE=SEDCE(IMO,I)
      IF(OCEAN.EQ.YES) CONSDO=SEDCO(IMO,I)
      IF(WATBOD.EQ.YES)CALL ALPHA(IMO,I)
C
C --- USE HYDROLOGIC CYCLE RESULTS TO CALULATE ANNUAL TOTALS AND
C --- AVERAGES
C
      DO 200 J=1,10
      HYDBAL(13,J)=HYDBAL(13,J)+HYDBAL(IMO,J)
  200 CONTINUE
      IF(IMO.EQ.12)HYDBAL(13,1)=HYDBAL(13,1)/12.
C
C --- PRINT HYDROLOGIC RESULTS
C
      IF(IMO.LT.12)GO TO 800
      WRITE(IOW,753) I
  753 FORMAT('1',5(/),25X,'YEAR -',I2,2X,'MONTHLY RESULTS (OUTPUT)',/,
     *25X,8('='),2X,24('='),/,/)
      WRITE(IOW,704)(AMO(IQ),IQ=1,12)
  704 FORMAT(5(/),6X,'-- HYDROLOGIC CYCLE COMPONENTS --',4(/),
     *18X,12(2X,A4,3X),/)
      DO 120  K=1,12
  120 HYDOUT(K)=HYDBAL(K,1)*100.
      WRITE(IOW,751)(HYDOUT(IMN),IMN=1,12),((HYDBAL(IMN,IVAL),IMN=1,12),
     *IVAL=2,5)
      WRITE(IOW,752)((HYDBAL(IMN,IVAL),IMN=1,12),IVAL=6,8)
  751 FORMAT(1X,'SOIL MOISTURE( %)',T20,12G9.3,/,
     *1X,'PRECIPATION(CM)',T20,12G9.3,/,
     *1X,'NET INFILTR.(CM)',T20,12G9.3,/,
     *1X,'EVAPOTRANSP.(CM)',T20,12G9.3,/,
     *1X,'SURFACE RUNOFF(CM)',T20,12G9.3)
  752 FORMAT(1X,'GRW RUNOFF(CM)',T20,12G9.3,/,
     *1X,'YIELD (CM)',T20,12G9.3,/,/,
     *1X,'RATIO PA/MPA(G%)',T20,12G9.3)
C
C --- DO MONTHLY POLLUTANT CYCLE  SIMULATION
C
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 800  CONTINUE
      DO 825 ISTEP=1,NSTEPS
      IF(LAKE.NE.YES.AND.RIVER.NE.YES.AND.ESTU.NE.YES.AND.OCEAN.EQ.YES)
     $    GO TO 600
C
C CALL AIR ROUTINE TO CALCULATE AIR CONCENTRATIONS; CONSIDERS INTERACTIONS
C BETWEEN AIR AND WATER AND BETWEEN AIR AND SOIL.
C
      CALL AIR(IMO,I,ISTEP,NSTEPS,DT)
      IPASS=1
      IF(WATBOD.EQ.NO)GO TO 500
C
C
      IF(LAKE.NE.YES) GO TO 300
      SWMINL=SWMOUL
C
C CONVERT WET & DRY DEPOSITION FROM AIR TO SOIL FROM KG/M**2/SEC
C   TO UG/CM**2/MON (NEXT TO LAKE)
C
      ASMIDL=ASMIDL*2.592E11
      ASMIWL=ASMIWL*2.592E11
      IWATER=1
C
C IWATER = 1 SIGNIFIES LAKE
C
      CALL TRANS3(I,IMO,ISTEP,NSTEPS,ASMIDL,ASMIWL,SURROF,
     $            GRWROF,SAMOUL,ARL,IWATER,IPASS,CUMLKE,CLMLKE,
     $            SUMLKE,SLMLKE,CUSALK,CLSALK,LIGCUL,LIGCLL,CMMLKE,
     $            SMMLKE,CMSALK,LIGCML)
      IPASS=2
C
C CALCULATE SOIL TO WATER RATE & CONVERT FROM MICRO-GRAMS/MON
C   TO KG/SEC
C
      SWMOUL=(SURROF+GRWROF)*3.8580247E-16
C
C CONVERT SOIL TO AIR RATE TO KG/SEC
C
      SAMOUL=SAMOUL*3.8580247E-16
C
C
  300 IF(RIVER.NE.YES) GO TO 400
      SWMINR=SWMOUR
C
C CONVERT WET & DRY DEPOSITION FROM AIR TO SOIL FROM
C  KG/M**2/SEC TO UG/CM**2/MON (NEXT TO RIVER)
C
      ASMIDR=ASMIDR*2.592E11
      ASMIWR=ASMIWR*2.592E11
      IWATER=2
C
C IWATER=2 SIGNIFIES RIVER
C
      CALL TRANS3(I,IMO,ISTEP,NSTEPS,ASMIDR,ASMIWR,SURROF,
     $            GRWROF,SAMOUR,ARR,IWATER,IPASS,CUMRIV,CLMRIV,
     $            SUMRIV,SLMRIV,CUSARV,CLSARV,LIGCUR,LIGCLR,CMMRIV,
     $              SMMRIV,CMSARV,LIGCMR)
      IPASS=2
C
C CALCULATE SOIL TO WATER RATE AND CONVERT FROM MICRO-GRAMS/MON
C  TO KG/SEC.
C
      SWMOUR=(SURROF+GRWROF)*3.8580247E-16
C
C CONVERT SOIL TO AIR RATE TO KG/SEC
C
      SAMOUR=SAMOUR*3.8580247E-16
C
C
  400 IF(ESTU.NE.YES) GO TO 600
      SWMINE=SWMOUE
C
C CONVERT WET & DRY DEPOSITION FROM AIR TO SOIL FROM
C  KG/M**2/SEC TO UG/CM**2/MON (NEXT TO ESTUARY)
C
      ASMIDE=ASMIDE*2.592E11
      ASMIWE=ASMIWE*2.592E11
      IWATER=3
C
C IWATER = 3 SIGNIFIES ESTUARY
C
      CALL TRANS3(I,IMO,ISTEP,NSTEPS,ASMIDE,ASMIWE,SURROF,
     $              GRWROF,SAMOUE,ARE,IWATER,IPASS,CUMEST,CLMEST,
     $              SUMEST,SLMEST,CUSAES,CLSAES,LIGCUE,LIGCLE,CMMEST,
     $              SMMEST,CMSAES,LIGCME)
      IPASS=2
C
C CALCULATE SOIL TO WATER RATE AND CONVERT FROM MICRO-GRAMS/MON
C  TO KG/SEC.
C
      SWMOUE=(SURROF+GRWROF)*3.8580247E-16
C
C CONVERT SOIL TO AIR RATE TO KG/SEC
C
      SAMOUE=SAMOUE*3.8580247E-16
      GO TO 600
 500  CONTINUE
C
C NO WATER BODY CONSIDERED, ONLY AIR & SOIL
C CONVERT WET AND DRY DEPOSITION FROM AIR TO SOIL FROM
C  KG/M**2/SEC TO UG/CM**2/MON
C
      ASMIDS=ASMIDS*2.592E11
      ASMIWS=ASMIWS*2.592E11
      IWATER=1
C
C IWATER = 1 AND WATBOD = NO SIGNIFIES NO WATER BODY
C
      CALL TRANS3(I,IMO,ISTEP,NSTEPS,ASMIDS,ASMIWS,SURROF,
     $              GRWROF,SAMOUS,ARS,IWATER,IPASS,CUMS,CLMS,
     $              SUMS,SLMS,CUSAS,CLSAS,LIGCUS,LIGCLS,CMMS,SMMS,
     $              CMSAS,LIGCMS)
```

```
      IPASS=2
C
C CONVERT SOIL TO AIR RATE TO KG/SEC
C
      SAMOUS=SAMOUS*3.8580247E-16
      GO TO 825
  600 CONTINUE
C
C CALL WATER SUBROUTINE FOR CALCULATION OF WATER CONCENTRATIONS (EACH WATER
C BODY), & INTERACTION TERMS BETWEEN WATER & AIR
C
      CALL WATER(INO,I,DT,ISTEP,NSTEPS)
 825  CONTINUE
C
C CALL FOODCHAIN ROUTINE
C
      CALL BIOCHN(INO,I)
C
C OUTPUT RESULTS
C
      CALL OUTPUT(INO,I)
  720 CONTINUE
C
C --- PRINT END MESSAGE
C
      WRITE(IOW,805)
  805 FORMAT(4(/),1X,40('*'),'EXECUTION COMPLETED',40('*'),/)
C
C --- RETURN TO MAIN PROGRAM
C
      RETURN
      END
      SUBROUTINE LINT(DI,ID1,IS,SO,VAL,IOW)
C
C --- THIS SUBROUTINE HAS BEEN CODED IN FORTRAN BY P.G. EAGLESON
C       (EAGLESON,1977)
C
C
C     THIS FUNCTION PRFORMS A LINEAR INTERPOLATION WHEN CALLED FROM
C     FUNTION FII(D,SO)
C
      DIMENSION DI(10,4)
      XX=SO-FLOAT(IS)*0.1
      Y1=DI(IS,ID1)
      Y2=DI(IS+1,ID1)
      VAL=(Y2-Y1)*10.*XX+Y1
      RETURN
      END
```

```
       SUBROUTINE RFILE
C      ================
C
C --- COMPILES USER INPUT DATA FROM DATA FILES
C
      REAL NUT1,LOAD
      COMMON /TI/ TITLES(5,12)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /HYM/ CLIMM1(6,12,10),CLIMM2(6,12,10),CLIMM3(12,10)
      COMMON /NU/ NUT1(6)
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12
      COMMON /HB/ HYDBAL(13,10)
      COMMON /FI/ IOR,IOW,IGE,IL0,IL1,IL2,IL3
      REAL LIGU,LIGM,LIGL,IA
      COMMON /LEV2/PCONC(13,15,3),THM,LIGU,LIGL,LIGM
      COMMON /HYR/ THA,PA,IA,ETA,RSA,RGA,YA,GZ,SIGMA,FGAM,G,XI
      DIMENSION TITLE(12),APPL(6),AJUNK(12)
C --- READ GENERAL DATA FILE
C --- (CLIMATALOGICAL,SOIL, CHEMISTRY,AND NUTRIENT DATA)
C
C --- READ SECTION TITLE
C
      READ(IGE,901)NF,NTY,TITLE
C
C --- CLIMATOLOGICAL DATA
C
  100 READ(IGE,902)NF,NRE,TITLE,IYRS,ITY
      IF(NF.EQ.2)GO TO 200
      IF(NF.EQ.3)GO TO 300
      IF(NF.EQ.4)GO TO 400
      IF(NF.EQ.9)GO TO 900
C
C --- IF NOT REGION SPECIFIED FOR THIS RUN, SKIP TO NEXT DATA  SET
C
      IF(NRE.NE.JRE)GO TO 150
C     WRITE(IOW,9021)NF,NRE,TITLE,IYRS,ITY
      DO 110 I=1,12
  110 TITLES(1,I)=TITLE(I)
C
C --- READ CLIMATOLOGICAL DATA- LEVEL 2,3
C
  130 DO 135 I=1,IYRS
      READ(IGE,906)(CLIMM1(1,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM1(2,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM1(3,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM1(4,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM1(5,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM1(6,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM2(1,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM2(2,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM2(3,IQ,I),IQ=1,12)
      READ(IGE,906)(CLIMM2(4,IQ,I),IQ=1,12)
      READ(IGE,906)(AJUNK(IQ),IQ=1,12)
  135 CONTINUE
```

```
      GO TO 100
C
C --- SKIP OVER REGIONAL DATA SET
C
  150 IEND=IYRS*11
      IF(IEND.EQ.0)IEND=4
      DO 160 I=1,IEND
      READ(IGE,904)
  160 CONTINUE
      GO TO 100
C
C --- SOIL DATA
C
  200 CONTINUE
  201 READ(IGE,901)NF,NSO,TITLE
      IF(NF.EQ.3)GO TO 300
      IF(NF.EQ.4)GO TO 400
      IF(NF.EQ.9)GO TO 900
C
C --- IF NOT SOIL TYPE SPECIFIED FOR THIS RUN, SKIP TO NEXT SOIL DATA
C     SET
C
      IF(NSO.NE.JSO)GO TO 250
      DO 210 I=1,12
  210 TITLES(2,I)=TITLE(I)
      READ(IGE,903)(SOIL1(IQ),IQ=1,6)
      READ(IGE,903)(SOIL2(IQ),IQ=1,6)
      GO TO 201
C
C --- SKIP OVER SOIL DATA SET
C
  250 DO 260 I=1,2
      READ(IGE,904)
  260 CONTINUE
      GO TO 201
C
C --- CHEMISTRY DATA
C
  300 CONTINUE
  301 READ(IGE,901)NF,NCH,TITLE
      IF(NF.EQ.4)GO TO 400
      IF(NF.EQ.9)GO TO 900
C
C --- IF NOT CHEMICAL SPECIFIED FOR THIS RUN, SKIP TO NEXT CHEMICAL
C     DATA SET
C
      IF(NCH.NE.JCH)GO TO 350
      DO 310 I=1,12
  310 TITLES(3,I)=TITLE(I)
      READ(IGE,903)(CHEM1(IQ),IQ=1,6)
      READ(IGE,903)(CHEM1(IQ),IQ=7,12)
      READ(IGE,903)(CHEM1(IQ),IQ=13,18)
      GO TO 301
C
C --- SKIP OVER CHEMICAL DATA SET
C
```

```
  350 DO 360 I=1,3
      READ(IGE,904)
  360 CONTINUE
      GO TO 301
C
C --- NUTRIENT DATA
C
  400 CONTINUE
  401 READ(IGE,901)NF,NNU,TITLE
      IF(NF.EQ.9)GO TO 900
C
C --- IF NOT NUTRIENT SET SPECIFIED FOR THIS RUN, SKIP TO NEXT
C     NUTRIENT DATA SET
C
      IF(NNU.NE.JNU)GO TO 450
      DO 410 I=1,12
  410 TITLES(4,I)=TITLE(I)
      READ(IGE,903)(NUT1(IQ),IQ=1,6)
      GO TO 401
C
C --- SKIP OVER NUTRIENT DATA SET
C
  450 READ(IGE,904)
      GO TO 401
C
C --- READ APPLICATION DATA FOR LEVEL OF THIS RUN
C
  900 IF(LEVEL.EQ.3)GO TO 1300
C
C --- LEVEL 3
C
 1300 READ(IL3,902)NF,NTY,TITLE,IYRS
      IF(NF.EQ.9)GO TO 999
C
C --- IF NOT APPLICATION SPECIFIED FOR THIS RUN, SKIP TO NEXT
C     APPLICATION DATA SET
C
      IF(NTY.NE.JAPPL)GO TO 1350
      DO 1310 I=1,12
 1310 TITLES(5,I)=TITLE(I)
      READ(IL3,903)(APPL(IQ),IQ=1,6)
      GEOM(1)=APPL(1)
      GEOM(2)=APPL(2)
      GEOM(3)=APPL(3)
      GEOM(4)=APPL(4)
      GEOM(14)=APPL(5)
      READ(IL3,903)(APPL(IQ),IQ=1,6)
      GEOM(15)=APPL(1)
      GEOM(16)=APPL(2)
      GEOM(17)=APPL(3)
      READ(IL3,903)(APPL(IQ),IQ=1,6)
      GEOM(6)=APPL(1)
      GEOM(9)=APPL(2)
      GEOM(7)=APPL(3)
      GEOM(10)=APPL(4)
      GEOM(8)=APPL(5)
      GEOM(11)=APPL(6)
      READ(IL3,903)(APPL(IQ),IQ=1,6)
      GEOM(18)=APPL(1)
      GEOM(19)=APPL(2)
      READ(IL3,906)(RUNM1(1,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(2,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(3,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(4,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(5,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(6,IQ),IQ=1,12)
      READ(IL3,906)(RUNM1(7,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(1,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(2,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(3,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(4,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(5,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(6,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(7,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(8,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(9,IQ),IQ=1,12)
      READ(IL3,906)(RUNM2(10,IQ),IQ=1,12)
      GO TO 999
C
C --- SKIP OVER OTHER LEVEL3 FILES
C
 1350 IF(IYRS.LE.0)IYRS=1
      IEND=21+((IYRS-1)*17)
      DO 1360 I=1,IEND
      READ(IL3,904)
 1360 CONTINUE
      GO TO 1300
C
C --- RETURN TO MAIN PROGRAM
C
  999 RETURN
C
  901 FORMAT(I1,1X,I3,1X,12A4)
  902 FORMAT(I1,1X,I3,1X,12A4,2I5)
 9011 FORMAT(1X,I1,1X,I3,1X,12A4)
 9021 FORMAT(1X,I1,1X,I3,1X,12A4,2I5)
  903 FORMAT(38X,6F7.2)
 9031 FORMAT(38X,6G7.2)
  904 FORMAT(1X)
  906 FORMAT(8X,12F6.2)
 9061 FORMAT(8X,12F6.2)
      END
      SUBROUTINE TRANS3(IYR,IMO,ISTEP,NSTEPS,ASMIND,ASMINW,SURROF,
     $                   GRWROF,SAMOUT,ARSPLU,IWATER,IPASS,CUM,
     $                   CLM,SUM,SLM,CUSA,CLSA,LIGCU,LIGCL,CMM,SMM,
     $                   CMSA,LIGCM)
C     ========== ======
C
C     THIS SUBROUTINE ESTIMATES THE MONTHLY POLLUTANT MASS DISTRIBUTION
C     IN A SOIL COMPARTMENT,CONSISTING OF 3 SOIL LAYERS.
C     SIMULATION STARTS WITH THE MONTH OF OCTOBER. CONCENTRATIONS AT
C     THE BEGINNING OF THE SIMULATION (IE THE COLUMN DOES NOT START
C     CLEAN) CAN BE INPUT.
C
C     THE THEORETICAL BACKGROUND IS DESCRIBED IN APPENDIX PT.
C
C
      REAL NUT1,LOAD
      COMMON /TI/ TITLES(5,12)
      COMMON /EX/ JRUN,LEVEL,JRE,JSO,JCH,JNUT,JAPPL,JYRS
      COMMON /HYM/ CLIMM1(6,12,10),CLIMM2(6,12,10),CLIMM3(12,10)
      COMMON /NU/ NUT1(6)
      COMMON /SO/ SOIL1(6),SOIL2(6)
      COMMON /CH/ CHEM1(18)
      COMMON /AP/ GEOM(20),LOAD(6),RUNL0(6),RUNM1(10,12),RUNM2(10,12)
      COMMON /HB/ HYDBAL(13,10)
      COMMON /FI/ IOR,IOW,IGE,IL0,IL1,IL2,IL3
      REAL LIGU,LIGM,LIGL,IA
      COMMON /LEV2/PCONC(13,15,3),THM,LIGU,LIGL,LIGM
      COMMON /HYR/ THA,PA,IA,ETA,RSA,RGA,YA,GE,SIGMA,FGAM,G,XI
      COMMON/FLAGS/AIRFLG,AIRPOL,TRICON,LAKE,RIVER,
     $             ESTU,OCEAN,SEDRIV,SEDLKE,DISFLG,CHMFLG,WATBOD
      COMMON/OUT/ACMAXL,AVAIRL,AVAIRR,AVAIRE,AWDEPL,AWDEPR,AWDEPE,
     $           ASDEPL,ASDEPR,ASDEPE,WVOLAL,WVOLAR,WVOLAE,SVOLAL,
     $           SVOLAR,SVOLAE,SWSURL,SWSURR,SWSURE,SWGRWL,SWGRWR,
     $           SWGRWE,SCONUL,SCONUR,SCONUE,SCONLL,SCONLR,SCONLE,
     $           CONL1,CONL2,CONL3,CONR1(20),CONR2(20),CONR3(20),
     $           CNCED1(11),CNCED2(11),CNCED3(11),CNCEU1(11),CNCEU2(11),
     $           CNCEU3(11),XESTY(11),CONO1(10),CONO2(10),CONO3(10),
     $           RESUSE,WASHL,WASHR,WASHE,ACMAXR,ACMAXE,ACMAXS,
     $           AVAIRS,ASDEPS,SVOLAS,SWGRWS,SCONUS,SCONLS,RESUSS,
     $           RESUSL,RESUSR,SCONML,SCONMR,SCONME,SCONMS,SWSURS,
     $           WASHS,AREA1(3)
      DIMENSION POLBAL(13,45,3),PINP(13,6,3)
      DIMENSION AMO(12),PINPU(3),PINPL(3),PINPM(3),AREA(3)
      REAL IM,KOC,MP,KDE,MPL,MPL1,MPO,MPLO,ISRM,INT,  N,
     $MWT,KNH,KBH,KAH,KTU,KTL,
     $MWTLIG,MWTML,NI,K1,K1E,K1U,K1L,KU,KL,K,LIGCU1,LIGCL1,
     $LIGCUF,LIGCLF,IMDU,KDEL,LIGCM,LIGCMF,KM,KDEM,K1M,IMDM,
     $MP2,MP2O,KTM,LIGCM1,LIGCU,LIGCL,K2
      REAL NO
      DATA AMO/' OCT',' NOV',' DEC',' JAN',' FEB',' MAR',
     *' APR',' MAY',' JUN',' JUL',' AUG',' SEP'/
      DATA ISKIP/1/,NO/4H  NO/
C
C --- INITIALIZE ARRAYS (SET ALL PLACES TO 0.0)
C
      IF(IMO.GT.1.OR.ISTEP.GT.1)GO TO 50
      DO 5 I=1,13
      DO 6 J=1,45
    6 POLBAL(I,J,IWATER)=0.0
      DO 7 J=1,6
    7 PINP(I,J,IWATER)=0.0
    5 CONTINUE
      DO 8 J=1,15
 8    PCONC(13,J,IWATER)=0.0
      LIGCUF=PCONC(12,10,IWATER)
      LIGCMF=PCONC(12,11,IWATER)
      LIGCLF=PCONC(12,12,IWATER)
C
C     CALCULATE ANNUAL PRECIPITATION MPASUM
C
      MPASUM=0.
      DO 9 IMON=1,12
 9    MPASUM=MPASUM+CLIMM2(1,IMON,IYR)
C
C     CONVERT MPASUM TO INCHES
C
      MPASUM=MPASUM*0.3937
C
C     CALCULATE SOIL EROSION G IN GRAMS OF SOIL/M**2/YEAR
C
      GWASH=7.0*(MPASUM**2.3)/(1.0+0.0007*(MPASUM**3.3))
C
C     CONVERT TO UNITS OF GRAMS/CM**2/MONTH
C
      GWASH=GWASH/(12.0*1.0E4)
C
C --- COMPILE GEOMETRY DATA
C
 10   IF(IYR.GT.1.OR.IMO.GT.1.OR.ISTEP.GT.1.OR.IPASS.GT.1)GO TO 50
      AR   = GEOM(1)
      Z    = GEOM(2)*100.
      DU   = GEOM(3)
      DM    = GEOM(4)
      A2KDE= GEOM(6)
      A2OC = GEOM(7)
      A2CC = GEOM(8)
      AKDE= GEOM(9)
      AOC = GEOM(10)
      ACC = GEOM(11)
      FRN = GEOM(14)
      PH  = GEOM(15)
      A2PH = GEOM(16)
      APH = GEOM(17)
      IF(PH.EQ.0.0)PH=7.0
      IF(A2PH.EQ.0.0)A2PH=1.0
      IF(APH.EQ.0.0)APH=1.0
      A2CEC= GEOM(18)
      ACEC= GEOM(19)
      DO 11 I=1,3
 11   AREA(I)=0.0
C
C --- COMPILE SOIL PARAMETERS
```

```
C
      RS = SOIL1(1)
      K1 = SOIL1(2)
      C  = SOIL1(3)
      N  = SOIL1(4)
      OC = SOIL1(5)
      CC = SOIL1(6)
      CEC= SOIL2(1)
      K1U= SOIL2(2)
      K1M= SOIL2(3)
      K1L= SOIL2(4)
      RDUST=SOIL2(5)
C
C --- SEDIMENT AND WIND SUSPENSION ROUTINES YET TO BE INCORPORATED
C
      SEDM=0.
      DUSTM=0.
C
C --- COMPILE CHEMISTRY DATA
C
      SL   = CHEM1(1)
      KOC  = CHEM1(2)
      DA   = CHEM1(3)
      KDE  = CHEM1(4)
      H    = CHEM1(5)
      K    = CHEM1(6)
      MWT  = CHEM1(7)
      VAL  = CHEM1(8)
      KNH  = CHEM1(9)
      KBH  = CHEM1(10)
      KAH  = CHEM1(11)
      SK   = CHEM1(13)
      B    = CHEM1(14)
      MWTLIG=  CHEM1(15)
C
C --- SET CONSTANTS
C
      R=8.2056E-5
      DT=30.
      NI=FLOAT(NSTEPS)
C
C --- SET INITIAL CONCENTRATIONS
C
      DPTH=DU
      LIGU=0.0
      LIGM=0.0
      LIGL=0.0
C
C --- SUPPORTING EQUATIONS:
C
C --- EQUATIONS FOR LOWER ZONES
C
   55 PHL=APH*PH
      OCL=OC*AOC
      CECL=CEC*ACEC
      KDEL=KDE*AKDE
      DL=Z-(DU+DM)
      PHM=A2PH*PH
      OCM=OC*A2OC
      CECM=CEC*A2CEC
      KDEM=KDE*A2KDE
C
C --- CALCULATE K FOR ORGANICS
C
      KU=K
      KM=K
      KL=K
      IF(KU.NE.0.)GO TO 16
      KU=KOC*OC/100.
      KM=KOC*OCM/100.
      KL=KOC*OCL/100.
C
C --- CALCULATE AVERAGE PERMEABILITY (IF NECESSARY)
C
   16 K1Z=K1
      IF(K1Z .NE. 0.0 )GO TO 20
C
C --- DIFFERENT PERMEABILITIES INPUT FOR EACH ZONE,CALCULATE AVE. PERM.
C
      K1Z=(DU+DM+DL)/((DU/K1U)+(DM/K1M)+(DL/K1L))
      GO TO 17
C
C --- SAME PERMEABILITY ENTERED FOR EACH ZONE
C
   20 K1U=K1Z
      K1M=K1Z
      K1L=K1Z
C
C --- CALCULATE TOTAL CATION EXCHANGE CAPACITY OF THE SOIL
C
   17 TCECU=0.0
      TCECM=0.0
      TCECL=0.0
      IF(VAL.EQ.0)GO TO 18
      TCECU=((CEC*MWT/VAL)*10.)*DU*RS
      TCECM=((CECM*MWT/VAL)*10.)*DM*RS
      TCECL=((CECL*MWT/VAL)*10.)*DL*RS
C
C --- CALCULATE MOLECULAR WEIGHT OF COMPLEX
C
   18 MWTML=MWT+B*MWTLIG
C
C --- CALCULATE HYDROLYSIS CONSTANTS
C
      KTU=0.0
      KTM=0.0
      KTL=0.0
      IF(KNH+KAH+KBH .EQ. 0.0) GO TO 21
      KTU=KNH+KAH*(10.**(-1.*PH))+KBH*(10.**(-1.*(14.-PH)))
      KTM=KNH+KAH*(10.**(-1.*PHM))+KBH*(10.**(-1.*(14.-PHM)))
      KTL=KNH+KAH*(10.**(-1.*PHL))+KBH*(10.**(-1.*(14.-PHL)))
C
```

```
C --- SET DEPTHS FOR VOLATILIZATION ROUTINE
C
   21 VOLDU=DU/2.
      VOLDM=DU+DM/2.
      VOLDL=DU+DM+DL/2.
C
C --- RUN FOR 12 MONTHS
C
 50   CONTINUE
C     WRITE(9,308)IYR,AMO(IMO),IMO
  308 FORMAT(1X,'YEAR',I5,5X,'MONTH',A4,2X,I2)
C
C --- COMPILE MONTHLY HYDROLOGIC PARAMETERS
C
      IF(ISTEP.GT.1.OR.ISKIP.GT.1)GO TO 40
      THM1= HYDBAL(IMO,1)
      PM  = HYDBAL(IMO,2)
      IM  = HYDBAL(IMO,3)
      EM  = HYDBAL(IMO,4)
      RSM = HYDBAL(IMO,5)
      RGM = HYDBAL(IMO,6)
C
C --- COMPILE MONTHLY APPLICATION DATA (LOADING,SURFACE RUNOFF,ETC.)
C
      POLINU = RUNM1(4,IMO)
      POLINM = RUNM1(5,IMO)
      POLINL = RUNM1(6,IMO)
      ISRM   = RUNM1(7,IMO)
      TA     = CLIMM1(2,IMO,IYR)
C
C --- COMPILE SECONDARY MONTHLY INPUT DATA
C
      ASL= RUNM2(1,IMO)
      TRANSU = RUNM2(2,IMO)/NI
      TRANSM = RUNM2(3,IMO)/NI
      TRANSL = RUNM2(4,IMO)/NI
      SINKU  = RUNM2(5,IMO)/NI
      SINKM  = RUNM2(6,IMO)/NI
      SINKL  = RUNM2(7,IMO)/NI
C
C --- ESTIMATE LOWER UNSZO INFILTRATION
C
      K2=(DU+DM)/((DU/K1U)+(DM/K1M))
      IMDU=(RGM+(IM-RGM)*((DM+DL)/Z))*(K1U/K1Z)
      IMDM=(RGM+(IM-RGM)*(DL/Z))*(K2/K1Z)
      ISKIP=2
 40   CONTINUE
      IF(ISTEP.EQ.NSTEPS)ISKIP=1
      IF(IPASS.GT.1)GO TO 45
      LIGU=LIGU+RUNM2(8,IMO)/NI
      LIGM=LIGM+RUNM2(9,IMO)/NI
      LIGL=LIGL+RUNM2(10,IMO)/NI
C
C --- CALCULATE LIGAND CONCENTRATION FROM LIGAND MASSES
C
      LIGCU1=LIGU/(DU*THM1)
      LIGCM1=LIGM/(DM*THM1)
      LIGCL1=LIGL/(DL*THM1)
C
C --- SEE IF GROUNDWATER CONTAMINATION IS POSSIBLE(I.E. IF ANY SURFACE
C     WATER FROM THIS SIMULATION REACHES THE GROUNDWATER THIS MONTH)
C     IF NOT SET GROUNDWATER RUNOFF TO ZERO FOR THIS MONTH'S
C     POLLUTANT CYCLE
C
      DPTH=DEPTH(THM1,N,IM,RGM,DPTH,NI)
      IF(DPTH.LE.Z)RGM=0.0
C
C --- ITERATIVE SOLUTION OF EQUATION SYSTEM -UPPER LAYER
C
C --- SET UP ITERATION PARAMETERS
C
 45   CONTINUE
      LAYER=1
      IFIG=0
      ISIG=0
      INT=1.E8
      SVCUM1=0.0
      CUM1=0.0
C
C --- TO START WITH A DIRTY SITE, LOAD CUM AND CLM
C
      IF(CUM.EQ.0.)CUM=RUNM1(1,IMO)
      IF(CMM.EQ.0.)CMM=RUNM1(2,IMO)
      IF(CLM.EQ.0.)CLM=RUNM1(3,IMO)
C
C --- SOLVE EQUATION SYSTEM-UPPER LAYER
C
      PINU=POLINU/NI + ASMIND/NI + ASMINW/NI
      PTHERU=CUM*THM*DU + SUM*RS*DU + CUSA*(N-THM)*DU + COMP(CUM,
     1 MWT,SK,LIGCU,MWTLIG,B,THM,DU)
C
C --- CALCULATE AMOUNT INVOLVED IN CEC
C
      IF(TCECU.GE.(PINU+PTHERU))PCECU=PINU+PTHERU
      IF(TCECU.LT.(PINU+PTHERU))PCECU=TCECU
      PHYDCU = PCECU*KTU*30./NI
      IF(PHYDCU .GT. PCECU)PHYDCU=PCECU
      PCECU=PCECU-PHYDCU
C
C --- CHECK VALID ENTRIES FOR OTHER SINKS AND TRANS
C
      IF(SINKU+TRANSU .LE. PINU+PTHERU-(PCECU+PHYDCU))GO TO 200
      SINKU=0.0
      TRANSU=0.0
      WRITE(IOW,806)IYR,IMO,ISTEP
 806  FORMAT(/,1X,'***WARNING-  YEAR',I5,' MONTH',I5,' ITERATION=',I5,
     *':',/,' INSUFFICIENT',
     *' POLLUTANT MASS FOR',/,' SPECIFIED SINKS AND TRANSFORMATIONS',
     *' IN UPPER ZONE',/,
     *' OTHER SINKS SET TO ZERO,OTHER TRANSFORMATIONS SET TO ZERO')
C
C --- MASS BALANCE EQUATION
```

```
C
  200 PREMU=THM1*CUM1*DU + CUM1**(1./FRN)*KU*RS*DU + PCECU +
     1COMP(CUM1,MWT,SK,LIGCU1,MWTLIG,B,THM1,DU) +
     2(CUM1*H*DU*(N-THM1))/(R*(TA+273.))
      POUTU = CUM1*RSM*ISRM/NI +
     $        VOLM(0.,CUM1,H,R,TA,VOLDU,DA,N,THM1,NI) +
     $        CUM1*IMDU/NI + SINKU +
     $        (CUM1**(1./FRN)*KU+PCECU/(RS+DU))*GWASH/NI
      PTRANU=CUM1*THM1*DU*KTU*30./NI
     $        + CUM1**(1./FRN)*DU*RS*KTU*KU*30./NI
     $        + CUM1*DU*THM1*KDE*30./NI
     $        + PHYDCU + TRANSU
C
C --- CONVERGENCE CRITERIA :BASED ON MP
C
      MP = PINU+PTHERU-PREMU-POUTU-PTRANU
C
C --- FIRST TIME THROUGH (CHECK FOR SPECIAL CASE OF CLEAN COLUMN)
C
      IF(CUM1) 300,300,305
  300 MPO=MP
      IF(ABS(MP).EQ. 0.00)GO TO 400
      SVCUM1=CUM1
      CUM1=CUM1+INT
      GO TO 200
C
C --- TEST FOR CONVERGENCE
C
  305 AMP=ABS(MP)
C
C --- CONVERGENCE CRITERION 1, IS EQUATION BALANCED WITHIN 1%
C
      IF(AMP.LT.1.E-8) GO TO 400
C
C --- CONVERGENCE CRITERION 2, HAS IT CROSSED THE ORIGIN(OVERSHOT)
C
      IF((MP*MPO).LT.0) GO TO 402
C
C --- CONVERGENCE CRITERION 3, IS IT GOING IN WRONG DIRECTION (I.E.
C     COLUMN HAS BECOME CLEAN IN THIS MONTH)
C
      IF(ABS(MPO).LT.ABS(MP))GO TO 401
C
C --- NOT CONVERGED
C
      IFIG=1
      SVCUM1=CUM1
      CUM1=CUM1+INT
      GO TO 200
C
C --- CROSSED ORIGIN, TRY SMALLER INTERVAL
C
  402 IF(IFIG .EQ. 0) GO TO 410
      ISIG=ISIG+1
      IF(ISIG.EQ.6)GO TO 409
  410 INT=INT/10.
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      IF(INT.LT. 1.E-16) GO TO 409
      CUM1=SVCUM1+INT
      GO TO 200
C
C --- SPECIAL CASE ALL POLLUTANT LEAVES THIS MONTH
C
  401 CUM1=0.
      GO TO 400
C
C ---STOP WHEN INTERVAL IS VERY SMALL,(I.E. CONCENTRATRATION IS
C    CALCULATED TO WITHIN NUMERICAL ACCURACY OF THE MACHINE)
C
  409 CUM1=SVCUM1
C
C --- FINAL CONVERGENCE OF UPPER LAYER-CALCULATE OTHER CONCENTRATIONS
C
  400 SUM1=(CUM1**(1./FRN)*DU*RS*KU + PCECU)/(RS*DU)
      CUSA1=(CUM1*H)/(R*(TA+273.))
      IF(MWT.EQ.0.0)GO TO 495
      LIGCUF=(LIGCU1*DU*THM1 - B*COMP(CUM1,MWT,SK,LIGCU1,MWTLIG,B,THM1,
     1DU )*(MWTLIG/MWT))/(DU*THM1)
      IF(LIGCUF.LT.0.)LIGCUF=0.0
C
C --- ITERATIVE SOLUTION OF EQUATION SYSTEM -MIDDLE LAYER
C
C --- SET UP ITERATION PARAMETERS
C
  495 LAYER=2
      IFIG=0
      ISIG=0
      INT=1.E8
      SVCMM1=0.0
      CMM1=0.0
C
C --- SOLVE EQUATION SYSTEM-MIDDLE LAYER
C
      PINM=POLINM/NI + CUM1*IMDU/NI
      PTHERM=CMM*THM*DM + SMM*RS*DM + CMSA*(N-THM)*DM + COMP(CMM,MWT,SK,
     1 LIGCM,MWTLIG,B,THM,DM)
C
C --- CALCULATE AMOUNT INVOLVED IN CEC
C
      IF(TCECM.GE.(PINM+PTHERM))PCECM=PINM+PTHERM
      IF(TCECM.LT.(PINM+PTHERM))PCECM=TCECM
      PHYDCM = PCECM*KTM*30./NI
      IF(PHYDCM .GT. PCECM)PHYDCM=PCECM
      PCECM=PCECM-PHYDCM
C
C --- CHECK THAT VALUES ENTERED FOR OTHER SINKS AND TRANS ARE VALID
C
      IF(SINKM+TRANSM .LE. PINM+PTHERM-(PCECM+PHYDCM))GO TO 500
      SINKM=0.0
      TRANSM=0.0
      WRITE(IOW,808)IYR,IMO,ISTEP
  808 FORMAT(/,1X,'***WARNING-  YEAR',I5,' MONTH',I5,' ITERATION=',I5,
     *':',/,' INSUFFICIENT',
     *' POLLUTANT MASS FOR',/,' SPECIFIED SINKS AND TRANSFORMATIONS',
     *' IN MIDDLE ZONE',/,
     *' OTHER SINKS SET TO ZERO,OTHER TRANSFORMATIONS SET TO ZERO')
C
C --- MASS BALANCE EQUATION
C
  500 PREMM=THM1*CMM1*DM + CMM1**(1./FRN)*KM*RS*DM + PCECM +
     1COMP(CMM1,MWT,SK,LIGCM1,MWTLIG,B,THM1,DM) +
     2(CMM1*H*DM*(N-THM1))/(R*(TA+273.))
      POUTM = CMM1*IMDM/NI +
     $        VOLM(CUM1,CMM1,H,R,TA,VOLDM,DA,N,THM1,NI) +
     $        SINKM
      PTRANM=CMM1*THM1*DM*KTM*30./NI
     $        + CMM1**(1./FRN)*DM*RS*KTM*KM*30./NI
     $        + CMM1*DM*THM1*KDEM*30./NI
     $        + PHYDCM + TRANSM
C
C --- CONVERGENCE CRITERIA :BASED ON MP2
C
      MP2= PINM+PTHERM-PREMM-POUTM-PTRANM
C
C --- FIRST TIME THROUGH (CHECK FOR SPECIAL CASE OF CLEAN COLUMN)
C
      IF(CMM1) 505,505,510
  505 MP2O=MP2
      IF(ABS(MP2).LT. 1.E-4)GO TO 590
      SVCMM1=CMM1
      CMM1=CMM1+INT
      GO TO 500
C
C --- TEST FOR CONVERGENCE
C
  510 AMP2=ABS(MP2)
C
C --- CONVERGENCE CRITERION 1, IS EQUATION BALANCED WITHIN 1%
C
      IF(AMP2.LT.0.01) GO TO 590
C
C --- CONVERGENCE CRITERION 2, HAS IT CROSSED THE ORIGIN(OVERSHOT)
C
      IF((MP2*MP2O).LT.0) GO TO 585
C
C --- CONVERGENCE CRITERION 3, IS IT GOING IN WRONG DIRECTION (SPECIAL
C     CASES)
C
      IF(ABS(MP2O).LT.ABS(MP2))GO TO 580
C
C --- NOT CONVERGED
C
      IFIG=1
      SVCMM1=CMM1
      CMM1=CMM1+INT
      GO TO 500
C
C --- CROSSED ORIGIN, TRY SMALLER INTERVAL
C
```

```
  585 IF(IFIG .EQ. 0) GO TO 575
      ISIG=ISIG+1
      IF(ISIG.EQ.6)GO TO 570
  575 INT=INT/10.
      IF(INT.LT. 1.E-8) GO TO 570
      CMM1=SVCMM1+INT
      GO TO 500
C
C --- SPECIAL CASE:
C --- ALL POLLUTANT LEAVES THIS MONTH
C
  580 CMM1=0.
      GO TO 590
C
C ---STOP WHEN INTERVAL IS VERY SMALL,(I.E. CONCENTRATRATION IS
C ---CALCULATED TO WITHIN NUMERICAL ACCURACY OF THE MACHINE)
C
  570 CMM1=SVCMM1
C
C --- FINAL CONVERGENCE OF MIDDLE LAYER-CALCULATE OTHER CONCENTRATIONS
C
  590 SMM1=(CMM1**(1./FRN)*DM*RS*KM + PCECM)/(RS*DM)
      CMSA1=(CMM1*H)/(R*(TA+273.))
      IF(MWT .EQ. 0) GO TO 599
      LIGCMF=(LIGCM1*DM*THM1 - B*COMP(CMM1,MWT,SK,LIGCM1,MWTLIG,B,THM1,
     1DM)*(MWTLIG/MWT))/(DM*THM1)
      IF(LIGCMF.LT.0.)LIGCMF=0.0
C
C --- ITERATIVE SOLUTION OF EQUATION SYSTEM -LOWER LAYER
C
C --- SET UP ITERATION PARAMETERS
C
  599 LAYER=3
      IFIG=0
      ISIG=0
      INT=1.E8
      SVCLM1=0.0
      CLM1=0.0
C
C --- SOLVE EQUATION SYSTEM-LOWER LAYER
C
      PINL=POLINL/NI + IMDM*CMM1/NI
      PTHERL=CLM*THM*DL + SLM*RS*DL + CLSA*(N-THM)*DL + COMP(CLM,MWT,SK,
     1 LIGCL,MWTLIG,B,THM,DL)
C
C --- CALCULATE AMOUNT INVOLVED IN CEC
C
      IF(TCECL.GE.(PINL+PTHERL))PCECL=PINL+PTHERL
      IF(TCECL.LT.(PINL+PTHERL))PCECL=TCECL
      PHYDCL = PCECL*KTL*30./NI
      IF(PHYDCL .GT. PCECL)PHYDCL=PCECL
      PCECL=PCECL-PHYDCL
C
C --- CHECK VALID ENTRIES FOR OTHER SINKS AND TRANS
C
      IF(SINKL+TRANSL .LE. PINL+PTHERL-(PCECL+PHYDCL))GO TO 600
      SINKL=0.0
      TRANSL=0.0
      WRITE(IOW,807)IYR,IMO,ISTEP
  807 FORMAT(/,1X,'***WARNING-  YEAR',I5,' MONTH',I5,' ITERATION=',I5,
     *':',/,' INSUFFICIENT',
     *' POLLUTANT MASS FOR',/,' SPECIFIED SINKS AND TRANSFORMATIONS',
     *' IN LOWER ZONE',/,
     *' OTHER SINKS SET TO ZERO,OTHER TRANSFORMATIONS SET TO ZERO')
C
C --- MASS BALANCE EQUATION
C
  600 PREML=THM1*CLM1*DL + CLM1**(1./FRN)*KL*RS*DL + PCECL +
     1COMP(CLM1,MWT,SK,LIGCL1,MWTLIG,B,THM1,DL) +
     2(CLM1*H*DL*(N-THM1))/(R*(TA+273.))
      CMAX=AMAX1(CUM1,CMM1)
      POUTL = CLM1*RGM/NI
     $        + VOLM(CMAX,CLM1,H,R,TA,VOLDL,DA,N,THM1,NI)
     $        + SINKL
      PTRANL=CLM1*THM1*DL*KTL*30./NI
     $        + CLM1**(1./FRN)*DL*RS*KTL*KL*30./NI
     $        + CLM1*DL*THM1*KDEL*30./NI
     $        + PHYDCL + TRANSL
C
C --- CONVERGENCE CRITERIA :BASED ON MPL1
C
      MPL1 = PINL+PTHERL-PREML-POUTL-PTRANL
C
C --- FIRST TIME THROUGH, (CHECK FOR SPECIAL CASE OF CLEAN COLUMN)
C
      IF(CLM1) 333,333,334
  333 MPLO=MPL1
      IF(ABS(MPL1).LT. 1.E-4) GO TO 444
      CLM1=CLM1+INT
      GO TO 600
C
C --- TEST FOR CONVERGENCE
C
  334 AMPL=ABS(MPL1)
C
C --- CONVERGENCE CRITERION 1, IS EQUATION BALANCED WITHIN 1%
C
      IF(AMPL.LT.0.01) GO TO 444
C
C --- CONVERGENCE CRITERION 2, HAS IT CROSSED THE ORIGIN(OVERSHOT)
C
      IF(MPL1*MPLO.LT.0.) GO TO 446
C
C --- CONVERGENCE CRITERION 3, IS IT GOING IN WRONG DIRECTION (I.E.
C     COLUMN HAS BECOME CLEAN IN THIS MONTH)
C
      IF(ABS(MPLO).LT.ABS(MPL1))GO TO 443
C
C --- NOT CONVERGED
C
      IFIG=1
      SVCLM1=CLM1
      CLM1=CLM1+INT
      GO TO 600
C
C --- CROSSED ORIGIN, TRY SMALLER INTERVAL
C
  446 IF(IFIG .EQ. 0) GO TO 450
      ISIG=ISIG+1
      IF(ISIG.EQ.6) GO TO 447
  450 INT=INT/10.
      IF(INT.LT.1.E-8) GO TO 447
      CLM1=SVCLM1+INT
      GO TO 600
C
C --- SPECIAL CASE ALL POLLUTANT LEAVES THIS MONTH
C
  443 CLM1=0.
      IF(RGM.EQ.0)GO TO 444
      PINFL=PINL+PTHERL
      GO TO 444
C
C ---STOP WHEN INTERVAL IS VERY SMALL
C
  447 CLM1=SVCLM1
C
C --- FINAL CONVERGENCE OF LOWER LAYER-CALCULATE SOIL CONCENTRATIONS
C
  444 SLM1=(CLM1**(1./FRN)*DL*RS*KL + PCECL)/(RS*DL)
      CLSA1=(CLM1*H)/(R*(TA+273.))
      IF(MWT .EQ. 0.0)GO TO 499
      LIGCLF=(LIGCL1*DL*THM1 - B*COMP(CLM1,MWT,SK,LIGCL1,MWTLIG,B,THM1,
     1DL)*(MWTLIG/MWT))/(DL*THM1)
      IF(LIGCLF .LT.0.)LIGCLF=0.0
  499 CONTINUE
C
C --- CALCULATE AND STORE MONTHLY POLLUTANT MASS DISTRIBUTIONS
C
C DEPTOT IS TOTAL DEPOSITION FROM DRY & WET DEPOSITION AND
C  DIRECT APPLICATION (POLINU)
C
      DEPTOT=ASMIND+ASMINW+POLINU+POLINM+POLINL
      IF(DEPTOT.EQ.0.0)GO TO 502
      DEPRAT=(ASMIND+ASMINW)/DEPTOT
      PINRAT=(POLINU+POLINM+POLINL)/DEPTOT
C
C AR IS AREA OF DIRECT APPLICATION, ARSPLU IS AREA OF SOIL AFFECTED
C BY DEPOSITION, AREASP IS WEIGHTED AREA
C
      AREASP=AR*PINRAT+ARSPLU*DEPRAT
      GO TO 504
 502  AREASP=AR
      IF(AREASP.EQ.0.0)AREASP=ARSPLU
 504  CONTINUE
      ARSPLU=AREASP
      IF(ARSPLU.EQ.0.0)GO TO 506
      AREA(IWATER)=ARSPLU
      GO TO 508
```

```
506   ARSPLU=AREA(IWATER)
508   CONTINUE
      PINP(IMO,1,IWATER)=PINP(IMO,1,IWATER)+ARSPLU*ASMINW/NI
      PINP(IMO,2,IWATER)=PINP(IMO,2,IWATER)+AR*POLINU/NI+ARSPLU*
     $                   ASMIND/NI
      PINP(IMO,3,IWATER)=PINP(IMO,3,IWATER)+AR*POLINL/NI
      PINP(IMO,4,IWATER)=PINP(IMO,4,IWATER)+AR*POLINM/NI
      PINP(IMO,6,IWATER)=0.0
      DO 350 I=1,5
      PINP(IMO,6,IWATER)=PINP(IMO,6,IWATER)+PINP(IMO,I,IWATER)
  350 CONTINUE
      POLBAL(IMO,1,IWATER)=POLBAL(IMO,1,IWATER)+AREASP*CUM1*RSM*ISRM/NI
      POLBAL(IMO,2,IWATER)=POLBAL(IMO,2,IWATER)+
     $   AREASP*VOLM(0.,CUM1,H,R,TA,VOLDU,DA,N,THM1,NI)
      POLBAL(IMO,3,IWATER)=POLBAL(IMO,3,IWATER)+AREASP*SINKU
      POLBAL(IMO,4,IWATER)=AREASP*(CUM1**(1./FRN))*RS*DU*KU
      POLBAL(IMO,5,IWATER)=POLBAL(IMO,5,IWATER)+
     $   AREASP*CUM1*THM1*DU*KDE*30./NI
      POLBAL(IMO,6,IWATER)=POLBAL(IMO,6,IWATER)+AREASP*TRANSU
      POLBAL(IMO,7,IWATER)=POLBAL(IMO,7,IWATER)+AREASP*CLM1*RGM/NI
      POLBAL(IMO,8,IWATER)=POLBAL(IMO,8,IWATER)+AREASP*SINKL
      POLBAL(IMO,9,IWATER)=AREASP*(CLM1**(1./FRN))*RS*DL*KL
      POLBAL(IMO,10,IWATER)=POLBAL(IMO,10,IWATER)+
     $   AREASP*CLM1*THM1*DL*KDEL*30./NI
      POLBAL(IMO,11,IWATER)=POLBAL(IMO,11,IWATER)+AREASP* TRANSL
      POLBAL(IMO,12,IWATER)=AREASP*THM1*CUM1*DU
      POLBAL(IMO,13,IWATER)=AREASP*THM1*CLM1*DL
      POLBAL(IMO,16,IWATER)=PCECU*AREASP
      POLBAL(IMO,17,IWATER)=PCECL*AREASP
      POLBAL(IMO,18,IWATER)=POLBAL(IMO,18,IWATER)+
     $   AREASP*CUM1*THM1*DU*KTU*30./NI
      POLBAL(IMO,19,IWATER)=POLBAL(IMO,19,IWATER)+
     $   AREASP*CLM1*THM1*DL*KTL*30./NI
      POLBAL(IMO,20,IWATER)=AREASP*
     $   COMP(CUM1,MWT,SK,LIGCU1,MWTLIG,B,THM1,DU)
      POLBAL(IMO,21,IWATER)=AREASP*
     $COMP(CLM1,MWT,SK,LIGCL1,MWTLIG,B,THM1,DL)
      POLBAL(IMO,22,IWATER)=POLBAL(IMO,22,IWATER) + AREASP*SINKM
      POLBAL(IMO,23,IWATER)=AREASP*(CMM1**(1./FRN))*RS*DM*KM
      POLBAL(IMO,24,IWATER)=POLBAL(IMO,24,IWATER)
     $                      +AREASP*CMM1*THM1*DM*KDEM*30./NI
      POLBAL(IMO,25,IWATER)=POLBAL(IMO,25,IWATER) + AREASP*TRANSM
      POLBAL(IMO,26,IWATER)=AREASP*THM1*CMM1*DM
      POLBAL(IMO,28,IWATER)=PCECM*AREASP
      POLBAL(IMO,29,IWATER)=POLBAL(IMO,29,IWATER)
     $                     +AREASP*CMM1*THM1*DM*KTM*30./NI
      POLBAL(IMO,30,IWATER)=AREASP*COMP(CMM1,MWT,SK,LIGCM1,MWTLIG,B,
     $                      THM1,DM)
      POLBAL(IMO,31,IWATER)=POLBAL(IMO,31,IWATER)+
     $                 AREASP*VOLM(CUM1,CMM1,H,R,TA,VOLDM,DA,N,THM1,NI)
      CMAX=AMAX1(CUM1,CMM1)
      POLBAL(IMO,32,IWATER)=POLBAL(IMO,32,IWATER)+AREASP*
     $VOLM(CMAX,CLM1,H,R,TA,VOLDL,DA,N,THM1,NI)
      POLBAL(IMO,33,IWATER)=POLBAL(IMO,33,IWATER)+AREASP*
     $(CUM1**(1./FRN))*KU*RS*DU*KTU*30./NI
      POLBAL(IMO,34,IWATER)=POLBAL(IMO,34,IWATER)+
     $AREASP*(CMM1**(1./FRN))*KM*RS*DM*KTM*30.0/NI
      POLBAL(IMO,35,IWATER)=POLBAL(IMO,35,IWATER)+AREASP*
     $(CLM1**(1./FRN))*KL*RS*DL*KTL*30./NI
      POLBAL(IMO,36,IWATER)=POLBAL(IMO,36,IWATER)+AREASP*PHYDCU
      POLBAL(IMO,37,IWATER)=POLBAL(IMO,37,IWATER)+AREASP*PHYDCM
      POLBAL(IMO,38,IWATER)=POLBAL(IMO,38,IWATER)+AREASP*PHYDCL
      POLBAL(IMO,39,IWATER)=AREASP*CUSA1*(N-THM1)*DU
      POLBAL(IMO,40,IWATER)=AREASP*CMSA1*(N-THM1)*DM
      POLBAL(IMO,41,IWATER)=AREASP*CLSA1*(N-THM1)*DL
      POLBAL(IMO,42,IWATER)=POLBAL(IMO,42,IWATER)+AREASP*SUM1*GWASH/NI
      PCONC(IMO,1,IWATER)=CUM1
      PCONC(IMO,2,IWATER)=CMM1
      PCONC(IMO,3,IWATER)=CLM1
      PCONC(IMO,4,IWATER)=SUM1
      PCONC(IMO,5,IWATER)=SMM1
      PCONC(IMO,6,IWATER)=SLM1
      PCONC(IMO,7,IWATER)=CUSA1
      PCONC(IMO,8,IWATER)=CMSA1
      PCONC(IMO,9,IWATER)=CLSA1
      PCONC(IMO,10,IWATER)=LIGCUF
      PCONC(IMO,11,IWATER)=LIGCMF
      PCONC(IMO,12,IWATER)=LIGCLF
      PCONC(IMO,13,IWATER)=DPTH
C
C --- THIS ITERATION'S CALCULATED CONCENTRATIONS BECOME STARTING
C     CONCENTRATIONS FOR THE NEXT ITERATION
C
      CUM=CUM1
      CMM=CMM1
      CLM=CLM1
      THM=THM1
      SUM=SUM1
      SMM=SMM1
      SLM=SLM1
      CUSA=CUSA1
      CMSA=CMSA1
      CLSA=CLSA1
      LIGCU=LIGCU1
      LIGCM=LIGCM1
      LIGCL=LIGCL1
C
C CALCULATE INTERACTION TERMS BETWEEN SOIL & WATER & AIR FOR
C WATER BODY I (USE WEIGHTED AREA FROM ABOVE - AREASP)
C I=1 SIGNIFIES LAKE, I=2 SIGNIFIES RIVER, I=3 SIGNIFIES ESTUARY
C I=1 AND WATBOD = NO SIGNIFIES NO WATER BODY IS CONSIDERED.
C SURROF INCLUDES BOTH WASHLOAD AND SURFACE RUNOFF
C
      SURROF=AREASP*(CUM1*RSM*ISRM+SUM1*GWASH)
      GRWROF=AREASP*CLM1*RGM
      IF(GRWROF.LT.0.)GRWROF=0.
      SAMOUT=AREASP*(VOLM(0.,CUM1,H,R,TA,VOLDU,DA,N,THM1,1.0)+
     $       VOLM(CUM1,CMM1,H,R,TA,VOLDM,DA,N,THM1,1.0)+
     $       VOLM(CMAX,CLM1,H,R,TA,VOLDL,DA,N,THM1,1.0))
      IF(ISTEP.LT.NSTEPS)RETURN
      IF(IWATER.EQ.1.AND.WATBOD.EQ.NO)GO TO 530
      IF(IWATER.NE.1)GO TO 610
      SVOLAL=POLBAL(IMO,2,IWATER)+POLBAL(IMO,31,IWATER)+
     $      POLBAL(IMO,32,IWATER)
      SWSURL=POLBAL(IMO,1,IWATER)
      SWGRWL=POLBAL(IMO,7,IWATER)
      SCONUL=(RS*SUM1+THM1*CUM1+(N-THM1)*CUSA1)*1.0E+6
      SCONML=(RS*SMM1+THM1*CMM1+(N-THM1)*CMSA1)*1.0E+6
      SCONLL=(RS*SLM1+THM1*CLM1+(N-THM1)*CLSA1)*1.0E+6
      RESUSL=RDUST*SUM1*1.E-6
      WASHL=POLBAL(IMO,42,IWATER)
 610  IF(IWATER.NE.2)GO TO 520
      SVOLAR=POLBAL(IMO,2,IWATER)+POLBAL(IMO,31,IWATER)+
     $      POLBAL(IMO,32,IWATER)
      SWSURR=POLBAL(IMO,1,IWATER)
      SWGRWR=POLBAL(IMO,7,IWATER)
      SCONUR=(RS*SUM1+THM1*CUM1+(N-THM1)*CUSA1)*1.0E+6
      SCONMR=(RS*SMM1+THM1*CMM1+(N-THM1)*CMSA1)*1.0E+6
      SCONLR=(RS*SLM1+THM1*CLM1+(N-THM1)*CLSA1)*1.0E+6
      RESUSR=RDUST*SUM1*1.E-6
      WASHR=POLBAL(IMO,42,IWATER)
 520  IF(IWATER.NE.3)GO TO 540
      SVOLAE=POLBAL(IMO,2,IWATER)+POLBAL(IMO,31,IWATER)+
     $      POLBAL(IMO,32,IWATER)
      SWSURE=POLBAL(IMO,1,IWATER)
      SWGRWE=POLBAL(IMO,7,IWATER)
      SCONUE=(RS*SUM1+THM1*CUM1+(N-THM1)*CUSA1)*1.0E+6
      SCONME=(RS*SMM1+THM1*CMM1+(N-THM1)*CMSA1)*1.0E+6
      SCONLE=(RS*SLM1+THM1*CLM1+(N-THM1)*CLSA1)*1.0E+6
      RESUSE=RDUST*SUM1*1.E-6
      WASHE=POLBAL(IMO,42,IWATER)
      GO TO 540
 530  SVOLAS=POLBAL(IMO,2,IWATER)+POLBAL(IMO,31,IWATER)+
     $      POLBAL(IMO,32,IWATER)
      SWSURS=POLBAL(IMO,1,IWATER)
      SWGRWS=POLBAL(IMO,7,IWATER)
      SCONUS=(RS*SUM1+THM1*CUM1+(N-THM1)*CUSA1)*1.0E+6
      SCONMS=(RS*SMM1+THM1*CMM1+(N-THM1)*CMSA1)*1.0E+6
      SCONLS=(RS*SLM1+THM1*CLM1+(N-THM1)*CLSA1)*1.0E+6
      RESUSS=RDUST*SUM1*1.E-6
      WASHS=POLBAL(IMO,42,IWATER)
 540  CONTINUE
C
C ---CALCULATE ANNUAL POLLUTANT MASS AVERAGES AND TOTALS
C
      DO 420 J=1,45
      POLBAL(13,J,IWATER)=POLBAL(13,J,IWATER)+POLBAL(IMO,J,IWATER)
  420 CONTINUE
      DO 430 J=1,6
      PINP(13,J,IWATER)=PINP(13,J,IWATER)+PINP(IMO,J,IWATER)
  430 CONTINUE
      DO 431 J=1,15
      PCONC(13,J,IWATER)=PCONC(13,J,IWATER)+PCONC(IMO,J,IWATER)
  431 CONTINUE
      IF(IMO.EQ.1)AREA1(IWATER)=AREASP*0.0001
      IF(IMO.LT.12)RETURN
      DO 432 J=1,15
 432  PCONC(13,J,IWATER)=PCONC(13,J,IWATER)/12.
```

```
      PINPU(IWATER) = PINP(13,1,IWATER) + PINP (13,2,IWATER)
      PINPM(IWATER) = PINP(13,4,IWATER)
      PINPL(IWATER) = PINP(13,3,IWATER)
C
C --- PRINT POLLUTANT CYCLE RESULTS
C
      WRITE(IOW,649)
 649  FORMAT(//,1X,T5,55('='),/)
      IF(IWATER.EQ.1.AND.WATBOD.EQ.NO)GO TO 695
      IF(IWATER.EQ.1) WRITE(IOW,650)
  650 FORMAT(/,1X,T5,'WATER BODY IS A LAKE')
      IF(IWATER.EQ.2) WRITE(IOW,670)
  670 FORMAT(/,1X,T5,'WATER BODY IS A RIVER')
      IF(IWATER.EQ.3) WRITE(IOW,690)
  690 FORMAT(/,1X,T5,'WATER BODY IS AN ESTUARY')
      GO TO 700
 695  WRITE(IOW,696)
 696  FORMAT(/,1X,T5,'THERE IS NO WATER BODY')
 700  CONTINUE
      WRITE(IOW,702)AREA1(IWATER)
 702  FORMAT(/,1X,T5,'CONTAMINATED SOIL AREA (1ST MONTH) IN M**2 = ',
     $1PE10.3)
      WRITE(IOW,649)
      WRITE(IOW,704)(AMO(IQ),IQ=1,12)
  704 FORMAT(5(/),
     *6X,'-- POLLUTANT MASS INPUT TO COLUMN(UG) --',
     *4(/),18X,12(2X,A4,3X),/)
      WRITE(IOW,751)((PINP(IQ,IVAL,IWATER),IQ=1,12),IVAL=1,2),
     *(PINP(IR,4,IWATER),IR=1,12),(PINP(IS,3,IWATER),IS=1,12)
      WRITE(IOW,753)(PINP(IQ,6,IWATER),IQ=1,12)
  751 FORMAT(1X,'PRECIPATION',T20,12G9.3,/,
     *1X,'OTHER(UPPER)',T20,12G9.3,/,
     *1X,'OTHER(MIDDLE)',T20,12G9.3,/,
     *1X,'OTHER(LOWER)',T20,12G9.3)
  753 FORMAT(/,/,1X,'TOTAL INPUT',T20,12G9.3)
      WRITE(IOW,705)
  705 FORMAT('1',/,6X,'-- POLLUTANT MASS DISTRIBUTION IN COLUMN (',
     *'UG) --')
      WRITE(IOW,706)
  706 FORMAT(2(/),1X,T5,'UPPER SOIL ZONE:',/)
      WRITE(IOW,759)((POLBAL(IQ,IVAL,IWATER),IQ=1,12),IVAL=1,4),
     *(POLBAL(IR,16,IWATER),IR=1,12)
  759 FORMAT(1X,'SURFACE RUNOFF',T20,12G9.3,/,
     *1X,'VOLATILIZED',T20,12G9.3,/,
     *1X,'OTHER SINKS',T20,12G9.3,/,
     *1X,'ADS. ON SOIL',T20,12G9.3,/,
     *1X,'IMMOBILIZED-CEC',T20,12G9.3)
      WRITE(IOW,762)(POLBAL(IQ,5,IWATER),IQ=1,12),
     *(POLBAL(IR,18,IWATER),IR=1,12),
     *(POLBAL(IT,33,IWATER),IT=1,12),
     *(POLBAL(IS,36,IWATER),IS=1,12),
     *(POLBAL(IS,20,IWATER),IS=1,12)
  762 FORMAT(1X,'DEGRADED',T20,12G9.3,/,
     *1X,'HYDROLYZED-MOI',T20,12G9.3,/,
     *1X,'HYDROLYZED-SOI',T20,12G9.3,/,
     *1X,'HYDROLYZED-CEC',T20,12G9.3,/,
   *1X,'COMPLEXED',T20,12G9.3)
    WRITE(IOW,763)(POLBAL(IQ,6,IWATER),IQ=1,12),
   *(POLBAL(IQ,12,IWATER),IQ=1,12),
   *(POLBAL(IR,39,IWATER),IR=1,12)
763 FORMAT(1X,'OTHER TRANS.',T20,12G9.3,
   */,1X,'IN SOIL MOIST.',T20,12G9.3,/,
   *1X,'IN SOIL AIR',T20,12G9.3)
    WRITE(IOW,720)
720 FORMAT(2(/),1X,T5,'MIDDLE SOIL ZONE:',/,/)
    WRITE(IOW,721)(POLBAL(IQ,31,IWATER),IQ=1,12),
   *(POLBAL(IR,22,IWATER),IR=1,12),
   *(POLBAL(IS,23,IWATER),IS=1,12),
   *(POLBAL(IT,28,IWATER),IT=1,12)
721 FORMAT(
   *1X,'VOLATILIZED',T20,12G9.3,/,
   *1X,'OTHER SINKS',T20,12G9.3,/,
   *1X,'ADS. ON SOIL',T20,12G9.3,/,
   *1X,'IMMOBILIZED-CEC',T20,12G9.3)
    WRITE(IOW,722)(POLBAL(IQ,24,IWATER),IQ=1,12),
   *(POLBAL(IR,29,IWATER),IR=1,12),
   *(POLBAL(IT,34,IWATER),IT=1,12),
   *(POLBAL(IS,37,IWATER),IS=1,12),
   *(POLBAL(IU,30,IWATER),IU=1,12)
722 FORMAT(1X,'DEGRADED',T20,12G9.3,/,
   *1X,'HYDROLYZED-MOI',T20,12G9.3,/,
   *1X,'HYDROLYZED-SOI',T20,12G9.3,/,
   *1X,'HYDROLYZED-CEC',T20,12G9.3,/,
   *1X,'COMPLEXED',T20,12G9.3)
    WRITE(IOW,723)(POLBAL(IQ,25,IWATER),IQ=1,12),
   *(POLBAL(IQ,26,IWATER),IQ=1,12),
   *(POLBAL(IR,40,IWATER),IR=1,12)
723 FORMAT(1X,'OTHER TRANS.',T20,12G9.3,
   */,1X,'IN SOIL MOIST.',T20,12G9.3,/,
   *1X,'IN SOIL AIR',T20,12G9.3)
    WRITE(IOW,764)
764 FORMAT(2(/),1X,T5,'LOWER SOIL ZONE:',/)
    WRITE(IOW,765)(POLBAL(IQ,7,IWATER),IQ=1,12),
   *(POLBAL(IQ,32,IWATER),IQ=1,12),
   *(POLBAL(IR,8,IWATER),IR=1,12),
   *(POLBAL(IT,9,IWATER),IT=1,12),
   *(POLBAL(IT,17,IWATER),IT=1,12),
   *(POLBAL(IS,10,IWATER),IS=1,12)
765 FORMAT(1X,'INTO GRWATER',T20,12G9.3,/,
   *1X,'VOLATILIZED',T20,12G9.3,/,
   *1X,'OTHER SINKS',T20,12G9.3,/,
   *1X,'ADS. ON SOIL',T20,12G9.3,/,
   *1X,'IMMOBILIZD-CEC',T20,12G9.3,/,
   *1X,'DEGRADED',T20,12G9.3)
    WRITE(IOW,766)(POLBAL(IQ,19,IWATER),IQ=1,12),
   *(POLBAL(IQ,35,IWATER),IQ=1,12),
   *(POLBAL(IQ,38,IWATER),IQ=1,12),
   *(POLBAL(IR,21,IWATER),IR=1,12),
   *(POLBAL(IT,11,IWATER),IT=1,12)
766 FORMAT(1X,'HYDROLYZED-MOI',T20,12G9.3,/,
   *1X,'HYDROLYZED-SOI',T20,12G9.3,/,
   *1X,'HYDROLYZED-CEC',T20,12G9.3,/,
     *1X,'COMPLEXED',T20,12G9.3,/,
     *1X,'OTHER TRANS.',T20,12G9.3)
      WRITE(IOW,760)(POLBAL(IU,13,IWATER),IU=1,12),
     *(POLBAL(IS,41,IWATER),IS=1,12)
760   FORMAT(
     *1X,'IN SOIL MOIST.',T20,12G9.3,/,
     *1X,'IN SOIL AIR',T20,12G9.3)
      WRITE(IOW,767)
767   FORMAT('1',3(/),6X,'-- POLLUTANT CONCENTRATIONS-(UG/ML) OR (UG/G)
     * --',/,/)
      WRITE(IOW,761)(PCONC(IQ,1,IWATER),IQ=1,12),
     *(PCONC(IR,4,IWATER),IR=1,12),
     *(PCONC(IR,7,IWATER),IR=1,12),
     *(PCONC(IT,10,IWATER),IT=1,12)
761   FORMAT(1X,'MOISTURE-UPPER',T20,12G9.3,/
     *1X,'SOIL-UPPER',T20,12G9.3,/,
     *1X,'AIR-UPPER',T20,12G9.3,/,
     *1X,'FREE LIGAND-UPPER',T20,12G9.3)
      WRITE(IOW,724)(PCONC(IQ,2,IWATER),IQ=1,12),
     *(PCONC(IR,5,IWATER),IR=1,12),
     *(PCONC(IR,8,IWATER),IR=1,12),
     *(PCONC(IT,11,IWATER),IT=1,12)
724   FORMAT(/,/,/,1X,'MOISTURE-MIDDLE',T20,12G9.3,/
     *1X,'SOIL-MIDDLE',T20,12G9.3,/,
     *1X,'AIR-MIDDLE',T20,12G9.3,/,
     *1X,'LIGAND-MIDDLE',T20,12G9.3)
      WRITE(IOW,770)(PCONC(IQ,3,IWATER),IQ=1,12),
     *(PCONC(IR,6,IWATER),IR=1,12),
     *(PCONC(IR,9,IWATER),IR=1,12),
     *(PCONC(IT,12,IWATER),IT=1,12)
770   FORMAT(/,/,1X,'MOISTURE-LOWER',T20,12G9.3,/
     *1X,'SOIL-LOWER',T20,12G9.3,/,
     *1X,'AIR-LOWER',T20,12G9.3,/,
     *1X,'FREE LIGAND-LOWER',T20,12G9.3)
      WRITE(IOW,768)(PCONC(IQ,13,IWATER),IQ=1,12)
768   FORMAT(/,/,1X,'MAX. POL.DEPTH(CM)',T20,12G9.3)
      WRITE(IOW,709)IYR
709   FORMAT('1',/,T30,'YEAR -',I5,'  ANNUAL SUMMARY REPORT',/,T30,
     *34('='))
      WRITE(IOW,714)PINPU(IWATER),PINPM(IWATER),PINPL(IWATER)
714   FORMAT(3(/),6X,'-- TOTAL INPUTS --',/,/,
     *1X,'UPPER SOIL ZONE',T35,G9.3,/,
     *1X,'MIDDLE SOIL ZONE',T35,G9.3,/,
     *1X,'LOWER SOIL ZONE',T35,G9.3)
      WRITE(IOW,710)
      HYDOUT=HYDBAL(13,1)*100
710   FORMAT(2(/),6X,'-- HYDROLOGIC CYCLE COMPONENTS --',/,/)
      WRITE(IOW,791)HYDOUT,(HYDBAL(13,IVAL),IVAL=2,5)
      WRITE(IOW,792)(HYDBAL(13,IVAL),IVAL=6,7)
791   FORMAT(1X,'AVERAGE SOIL MOISTURE( %)',T35,G9.3,/,
     *1X,'TOTAL PRECIPATION(CM)',T35,G9.3,/,
     *1X,'TOTAL INFILTRATION (CM)',T35,G9.3,/,
     *1X,'TOTAL EVAPOTRANSP.(CM)',T35,G9.3,/,
     *1X,'TOTAL SURFACE RUNOFF(CM)',T35,G9.3)
792   FORMAT(1X,'TOTAL GRW RUNOFF(CM)',T35,G9.3,/,
     *1X,'TOTAL YIELD (CM)',T35,G9.3,/)
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      WRITE(IOW,780)
  780 FORMAT(/,/,6X,'-- POLLUTANT MASS DISTRIBUTION (UG) --',/,/,
     *1X,3X,'UPPER SOIL ZONE:',/,/)
      WRITE(IOW,771)(POLBAL(13,IVL,IWATER),IVL=1,3),POLBAL(12,4,IWATER),
     *POLBAL(12,16,IWATER)
  771 FORMAT(1X,'TOTAL SURFACE RUNOFF',T35,G9.3,/,
     *1X,'TOTAL VOLATILIZED',T35,G9.3,/,
     *1X,'TOTAL OTHER SINKS',T35,G9.3,/,
     *1X,'FINAL ADS. ON SOIL',T35,G9.3,/,
     *1X,'FINAL IMMOBILIZED-CEC',T35,G9.3)
      WRITE(IOW,772)POLBAL(13,5,IWATER),
     *POLBAL(13,18,IWATER),
     *POLBAL(13,33,IWATER),
     *POLBAL(13,36,IWATER),
     *POLBAL(12,20,IWATER)
  772 FORMAT(1X,'TOTAL DEGRADED',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-MOI',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-SOI',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-CEC',T35,G9.3,/,
     *1X,'FINAL COMPLEXED',T35,G9.3)
      WRITE(IOW,773)POLBAL(13,6,IWATER),
     *POLBAL(12,12,IWATER),
     *POLBAL(12,39,IWATER)
  773 FORMAT(1X,'TOTAL OTHER TRANS.',T35,G9.3,
     */,1X,'FINAL IN SOIL MOIST.',T35,G9.3,/,
     *1X,'FINAL IN SOIL AIR',T35,G9.3)
      WRITE(IOW,730)
  730 FORMAT(2(/),1X,T5,'MIDDLE SOIL ZONE:',/,/)
      WRITE(IOW,725)POLBAL(13,31,IWATER),POLBAL(13,22,IWATER),
     *POLBAL(12,23,IWATER),
     *POLBAL(12,28,IWATER)
  725 FORMAT(
     *1X,'TOTAL VOLATILIZED',T35,G9.3,/,
     *1X,'TOTAL OTHER SINKS',T35,G9.3,/,
     *1X,'FINAL ADS. ON SOIL',T35,G9.3,/,
     *1X,'FINAL IMMOBILIZED-CEC',T35,G9.3)
      WRITE(IOW,726)POLBAL(13,24,IWATER),
     *POLBAL(13,29,IWATER),
     *POLBAL(13,34,IWATER),
     *POLBAL(13,37,IWATER),
     *POLBAL(12,30,IWATER)
  726 FORMAT(1X,'TOTAL DEGRADED',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-MOI',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-SOI',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-CEC',T35,G9.3,/,
     *1X,'FINAL COMPLEXED',T35,G9.3)
      WRITE(IOW,727)POLBAL(13,25,IWATER),
     *POLBAL(12,26,IWATER),
     *POLBAL(12,40,IWATER)
  727 FORMAT(1X,'TOTAL OTHER TRANS.',T35,G9.3,
     */,1X,'FINAL IN SOIL MOIST.',T35,G9.3,/,
     *1X,'FINAL IN SOIL AIR',T35,G9.3)
      WRITE(IOW,764)
      WRITE(IOW,774)POLBAL(13,7,IWATER),
     *POLBAL(13,32,IWATER),
     *POLBAL(13,8,IWATER),
     *POLBAL(12,9,IWATER),
     *POLBAL(12,17,IWATER),
     *POLBAL(13,10,IWATER)
  774 FORMAT(1X,'TOTAL INTO GRWATER',T35,G9.3,/,
     *1X,'TOTAL VOLATALIZED',T35,G9.3,/,
     *1X,'TOTAL OTHER SINKS',T35,G9.3,/,
     *1X,'FINAL ADS. ON SOIL',T35,G9.3,/,
     *1X,'FINAL IMMOBILIZED-CEC',T35,G9.3,/,
     *1X,'TOTAL DEGRADED',T35,G9.3)
      WRITE(IOW,775)POLBAL(13,19,IWATER),
     *POLBAL(13,35,IWATER),
     *POLBAL(13,38,IWATER),
     *POLBAL(12,21,IWATER),
     *POLBAL(13,11,IWATER)
  775 FORMAT(1X,'TOTAL HYDROLYZED-MOI',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-SOI',T35,G9.3,/,
     *1X,'TOTAL HYDROLYZED-CEC',T35,G9.3,/,
     *1X,'FINAL COMPLEXED',T35,G9.3,/,
     *1X,'TOTAL OTHER TRANS.',T35,G9.3)
      WRITE(IOW,776)POLBAL(12,13,IWATER),
     *POLBAL(12,41,IWATER)
  776 FORMAT(
     *1X,'FINAL IN SOIL MOIST.',T35,G9.3,/,
     *1X,'FINAL IN SOIL AIR',T35,G9.3)
      WRITE(IOW,777)
  777 FORMAT('1',5(/),6X,'-- AVERAGE POLLUTANT CONCENTRATIONS-(UG/ML)'
     *,'OR (UG/G) --',/,/)
      WRITE(IOW,781)PCONC(13,1,IWATER),
     *PCONC(13,4,IWATER),
     *PCONC(13,7,IWATER),
     *PCONC(13,10,IWATER)
  781 FORMAT(/,/,/,1X,'MOISTURE-UPPER',T35,G9.3,/
     *1X,'SOIL-UPPER',T35,G9.3,/,
     *1X,'AIR-UPPER',T35,G9.3,/,
     *1X,'FREE LIGAND-UPPER',T35,G9.3)
      WRITE(IOW,728)PCONC(13,2,IWATER),
     *PCONC(13,5,IWATER),
     *PCONC(13,8,IWATER),
     *PCONC(13,11,IWATER)
  728 FORMAT(/,/,/,1X,'MOISTURE-MIDDLE',T35,G9.3,/
     *1X,'SOIL-MIDDLE',T35,G9.3,/,
     *1X,'AIR-MIDDLE',T35,G9.3,/,
     *1X,'FREE LIGAND-MIDDLE',T35,G9.3)
      WRITE(IOW,779)PCONC(13,3,IWATER),
     *PCONC(13,6,IWATER),
     *PCONC(13,9,IWATER),
     *PCONC(13,12,IWATER)
  779 FORMAT(/,/,/,1X,'MOISTURE-LOWER',T35,G9.3,/
     *1X,'SOIL-LOWER',T35,G9.3,/,
     *1X,'AIR-LOWER',T35,G9.3,/,
     *1X,'FREE LIGAND-LOWER',T35,G9.3)
      PDEP=PCONC(12,13,IWATER)/100.
      WRITE(IOW,778)PDEP
  778 FORMAT(/,1X,'MAX. POL. DEPTH(M)',T35,G9.3)
C
C --- RETURN TO LEVEL ROUTINES
```

```
C
  999 RETURN
      END
      FUNCTION VOLM(C1,C2,H,R,T,DPTH,DA,N,THA,NI)
C
C     THIS FUNCTION CALCULATES THE POLLUTANT MASS (UG/SQ CM) INVOLVED
C     IN VOLATILIZATION FOR THE MONTLY ROUTINES
C
      REAL N,NI
C
C --- CHECK CONCENTRATION GRADIENT
C
      VOLM=0.0
      IF(C1 .GE. C2) GO TO 10
      VOLM=C2*(H/(R*(T+273.)*DPTH))*DA*((N-THA)**(10./3.)/N**2)
     2 *86400.*30/NI
   10 RETURN
      END
      SUBROUTINE WATCN(TA,SUT,NU,GAMSW)
C     ================
C
C --- THIS SUBROUTINE HAS BEEN CODED IN FORTRAN BY P.G. EAGLESON
C        (EAGLESON,1977)
C
C
C     COMPUTES THE WATER CONSTANTS AT A GIVEN TEMPERATURE(EAGLESON,1977)
      REAL NU,NUT
      DIMENSION SUTT(11),NUT(11),GAMST(11)
      DATA SUTT/75.6,74.9,74.2,73.5,72.0,72.1,71.4,70.7,70.0,69.3,68.6/,
     1 NUT/17.93E-3,15.18E-3,13.09E-3,11.44E-3,10.08E-3,8.94E-3,8.E-3,
     27.2E-3,6.53E-3,5.97E-3,5.94E-3/,
     3GAMST/0.99987,0.99999,0.99973,0.99913,0.99823,0.99708,0.99568,0.99
     4406,0.99225,0.99025,0.98807/
      IF(TA.GT.50.) GO TO 10
      ITA=IFIX(TA*0.2)+1
      FRAC=TA-FLOAT(IFIX(TA))
      ITA1=ITA+1
      SUT=(SUTT(ITA1)-SUTT(ITA))*0.2*FRAC+SUTT(ITA)
      NU=(NUT(ITA1)-NUT(ITA))*0.2*FRAC+NUT(ITA)
      GAMSW=((GAMST(ITA1)-GAMST(ITA))*0.2*FRAC+GAMST(ITA))*980.
      RETURN
   10 SUT=SUTT(11)
      NU=NUT(11)
      GAMSW=GAMST(11)*980.
      RETURN
      END
```

The following routines comprise the general purpose integrator package D01AJF.

```
      SUBROUTINE D01AJF(F, A, B, EPSABS, EPSREL, RESULT, ABSERR,
     * WORK, LWORK, IWORK, LIWORK, IFAIL)
C     MARK 8 RELEASE. NAG COPYRIGHT 1980
C
C     D01AJF IS A GENERAL PURPOSE INTEGRATOR WHICH CALCULATES
C     AN APPROXIMATION TO THE INTEGRAL OF A FUNCTION OVER A FINITE
C     INTERVAL (A,B)
C
C     D01AJF ITSELF IS ESSENTIALLY A DUMMY ROUTINE WHOSE FUNCTION IS TO
C     PARTITION THE WORK ARRAYS WORK AND IWORK FOR USE BY D01AJV.
C     WORK IS PARTITIONED INTO 4 ARRAYS EACH OF SIZE LWORK/4.
C     IWORK IS A SINGLE ARRAY IN D01AJV.
C
C     .. SCALAR ARGUMENTS ..
      REAL A, ABSERR, B, EPSABS, EPSREL, RESULT
      INTEGER IFAIL, LIWORK, LWORK
C     .. ARRAY ARGUMENTS ..
      REAL WORK(LWORK)
      INTEGER IWORK(LIWORK)
C     .. FUNCTION ARGUMENTS ..
      REAL F
C     ..
C     .. LOCAL SCALARS ..
      DOUBLE PRECISION SRNAME
      INTEGER IBL, IEL, IER, IRL, LIMIT
C     .. FUNCTION REFERENCES ..
      INTEGER P01AAF
C     .. SUBROUTINE REFERENCES ..
C     D01AJV
C     ..
      EXTERNAL F
      DATA SRNAME /8H D01AJF /
C     CHECK THAT MINIMUM WORKSPACE REQUIREMENTS ARE MET
      IF (LWORK.LT.4) GO TO 20
      IF (LIWORK.LT.LWORK/8+2) GO TO 20
C     LIMIT = UPPER BOUND ON NUMBER OF SUBINTERVALS
      LIMIT = LWORK/4
C     SET UP BASE ADDRESSES FOR WORK ARRAYS
      IBL = LIMIT + 1
      IEL = LIMIT + IBL
      IRL = LIMIT + IEL
C     PERFORM INTEGRATION
      CALL D01AJV(F, A, B, ABS(EPSABS), ABS(EPSREL), WORK(1),
     * WORK(IBL), WORK(IEL), WORK(IRL), LIMIT, IWORK, LIWORK,
     * RESULT, ABSERR, IER)
      IF (IER.NE.0) GO TO 40
      IFAIL = 0
      GO TO 60
C     ERROR 6 = INSUFFICIENT WORKSPACE
   20 IER = 6
   40 IFAIL = P01AAF(IFAIL,IER,SRNAME)
   60 RETURN
      END
      SUBROUTINE D01AJV(F, A, B, EPSABS, EPSREL, ALIST, BLIST,
     * ELIST, RLIST, LIMIT, IORD, LIORD, RESULT, ABSERR, IER)
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
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C     BASED ON QUADPACK ROUTINE DQAGS (FORMERLY QAGS)
C     ***********************************************************
C
C        PURPOSE
C           THE ROUTINE CALCULATES AN APPROXIMATION
C           /RESULT/ TO A GIVEN DEFINITE INTEGRAL   I =
C           INTEGRAL OF /F/ OVER (A,B), HOPEFULLY
C           SATISFYING FOLLOWING CLAIM FOR ACCURACY .
C           ABS(I-RESULT) .LE. MAX(EPSABS,EPSREL*ABS(I)).
C
C          CALLING SEQUENCE
C           CALL D01AJV (F,A,B,EPSABS,EPSREL,ALIST,BLIST,ELIST,
C                        RLIST,LIMIT,IORD,LIORD,RESULT,ABSERR,IER)
C
C        PARAMETERS
C            F      - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND
C                     FUNCTION F(X). THE ACTUAL NAME FOR F
C                     NEEDS TO BE DECLARED E X T E R N A L
C                     IN THE DRIVER PROGRAM
C
C            A      - LOWER LIMIT OF INTEGRATION
C
C            B      - UPPER LIMIT OF INTEGRATION
C
C            EPSABS - ABSOLUTE ACCURACY REQUESTED
C
C            EPSREL - RELATIVE ACCURACY REQUESTED
C
C            ALIST,BLIST,ELIST,RLIST
C                   - WORK ARRAYS (FUNCTIONS DESCRIBED BELOW)
C
C            LIMIT  - UPPER BOUND FOR NUMBER OF SUBINTERVALS
C
C            IORD   - WORK ARRAY
C
C            LIORD  - LENGTH OF IORD (AT LEAST LIMIT/2 + 2)
C
C            RESULT - APPROXIMATION TO THE INTEGRAL
C
C            ABSERR - ESTIMATE OF THE MODULUS OF THE ABSOLUTE ERROR,
C                     WHICH SHOULD EQUAL OR EXCEED ABS(I-RESULT)
C
C            IER    - IER   = 0 NORMAL AND RELIABLE
C                             TERMINATION OF THE ROUTINE.
C                             IT IS ASSUMED THAT THE
C                             REQUESTED  ACCURACY HAS BEEN
C                             ACHIEVED.
C                   - IER   .NE. 0 ABNORMAL TERMINATION OF
C                             THE ROUTINE. THE ESTIMATES
C                             FOR INTEGRAL AND ERROR ARE
C                             LESS RELIABLE. IT IS ASSUMED
C                             THAT THE  REQUESTED ACCURACY
C                             HAS NOT BEEN ACHIEVED.
C                         = 1 MAXIMUM NUMBER OF SUBDIVISIONS ALLOWED
C                             HAS BEEN ACHIEVED. THE USER CAN
C                             ALLOW MORE SUB DIVISIONS BY
```

```
C                             INCREASING THE DIMENSIONS OF THE
C                             WORK ARRAYS WORK AND IWORK.
C                             HOWEVER, THIS MAY
C                             YIELD NO  IMPROVEMENT, AND IT
C                             IS RATHER ADVISED TO HAVE A
C                             CLOSE LOOK AT THE INTEGRAND,
C                             IN ORDER TO DETERMINE THE
C                             INTEGRATION  DIFFICULTIES. IF
C                             THE POSITION OF A LOCAL
C                             DIFFICULTY CAN BE DETERMINED
C                             (I.E.  SINGULARITY,
C                             DISCONTINUITY WITHIN THE
C                             INTERVAL) ONE WILL PROBABLY
C                             GAIN FROM  SPLITTING UP THE
C                             INTERVAL AT THIS POINT AND
C                             CALLING THE INTEGRATOR ON THE
C                             SUB-RANGES. IF POSSIBLE, AN
C                             APPROPRIATE SPECIAL-PURPOSE
C                             INTEGRATOR SHOULD BE USED
C                             WHICH IS DESIGNED FOR
C                             HANDLING THE TYPE  OF
C                             DIFFICULTY INVOLVED.
C                         = 2 THE OCCURRENCE OF ROUNDOFF
C                             ERROR IS DETECTED WHICH
C                             PREVENTS THE REQUESTED
C                             TOLERANCE  FROM BEING
C                             ACHIEVED. THE ERROR MAY BE
C                             UNDER-ESTIMATED.
C                         = 3 EXTREMELY BAD INTEGRAND BEHAVIOUR
C                             OCCURS AT SOME INTERIOR POINTS OF THE
C                             INTEGRATION INTERVAL.
C                         = 4 IT IS PRESUMED THAT THE REQUESTED
C                             TOLERANCE CANNOT BE ACHIEVED,
C                             AND THAT THE RETURNED RESULT
C                             IS THE BEST WHICH CAN BE
C                             OBTAINED.
C                         = 5 THE INTEGRAL IS PROBABLY DIVERGENT, OR
C                             SLOWLY CONVERGENT. IT MUST BE NOTED
C                             THAT DIVERGENCY CAN OCCUR
C                             WITH ANY OTHER VALUE OF IER.
C
C     **********************************************************
C     .. SCALAR ARGUMENTS ..
      REAL A, ABSERR, B, EPSABS, EPSREL, RESULT
      INTEGER IER, LIMIT, LIORD
C     .. ARRAY ARGUMENTS ..
      REAL ALIST(LIMIT), BLIST(LIMIT), ELIST(LIMIT), RLIST(LIMIT)
      INTEGER IORD(LIORD)
C     .. FUNCTION ARGUMENTS ..
      REAL F
C     ..
C     .. SCALARS IN COMMON ..
      INTEGER JUPBND
C     ..
C     .. LOCAL SCALARS ..
      REAL A1, A2, ABSEPS, AREA12, AREA1, AREA2, AREA, B1, B2,
     * CORREC, DEFAB1, DEFAB2, DEFABS, DRES, EPMACH, ERLARG,
     * ERLAST, ERRBND, ERRMAX, ERRO12, ERROR1, ERROR2, ERRSUM,
     * ERTEST, OFLOW, RESABS, RESEPS, SMALL, UFLOW
      INTEGER ID, IERRO, IROFF1, IROFF2, IROFF3, K, KSGN, KTMIN,
     * LAST1, LAST, MAXERR, NRES, NRMAX, NUMRL2
      LOGICAL EXTRAP, NOEXT
C     .. LOCAL ARRAYS ..
      REAL RES3LA(3), RLIST2(52)
C     .. FUNCTION REFERENCES ..
      REAL X02AAF, X02ABF, X02ACF
C     .. SUBROUTINE REFERENCES ..
C     D01AJX, D01AJY, D01AJZ
C     ..
      EXTERNAL F
      COMMON /AD01AJ/ JUPBND
C
C            THE DIMENSION OF /RLIST2/ IS DETERMINED BY
C            DATA /LIMEXP/ IN SUBROUTINE D01AJY (/RLIST2/
C            SHOULD BE OF DIMENSION (LIMEXP+2) AT LEAST).
C
      EPMACH = X02AAF(1.0)
      UFLOW = X02ABF(1.0)
      OFLOW = X02ACF(1.0)
C
C            LIST OF MAJOR VARIABLES
C            -----------------------
C
C           ALIST     - LIST OF LEFT END-POINTS OF ALL SUBINTERVALS
C                       CONSIDERED UP TO NOW
C
C           BLIST     - LIST OF RIGHT END-POINTS OF ALL SUBINTERVALS
C                       CONSIDERED UP TO NOW
C
C           RLIST(I)  - APPROXIMATION TO THE INTEGRAL OVER
C                       (ALIST(I),BLIST(I))
C
C           RLIST2    - ARRAY OF DIMENSION AT LEAST LIMEXP+2
C                       CONTAINING THE PART OF THE EPSILON TABLE
C                       WHICH IS STILL NEEDED FOR FURTHER
C                       COMPUTATIONS
C
C           ELIST(I)  - ERROR ESTIMATE APPLYING TO RLIST(I)
C
C           MAXERR    - POINTER TO THE INTERVAL WITH LARGEST ERROR
C                       ESTIMATE
C
C           ERRMAX    - ELIST(MAXERR)
C
C           ERLAST    - ERROR ON THE INTERVAL CURRENTLY SUBDIVIDED
C                       (BEFORE THAT SUBDIVISION HAS TAKEN PLACE)
C
C           AREA      - SUM OF THE INTEGRALS OVER THE SUBINTERVALS
C
C           ERRSUM    - SUM OF THE ERRORS OVER THE SUBINTERVALS
C
C           ERRBND    - REQUESTED ACCURACY MAX(EPSABS,EPSREL*
C                 ABS(RESULT))
C
C           *****1    - VARIABLE FOR THE LEFT INTERVAL
C
C           *****2    - VARIABLE FOR THE RIGHT INTERVAL
C
C           LAST      - INDEX FOR SUBDIVISION
C
C           NRES      - NUMBER OF CALLS TO THE EXTRAPOLATION ROUTINE
C
C           NUMRL2    - NUMBER OF ELEMENTS CURRENTLY  IN
C                       RLIST2. IF AN APPROPRIATE
C                       APPROXIMATION TO THE COMPOUNDED
C                       INTEGRAL HAS BEEN OBTAINED IT IS
C                       PUT IN  RLIST2(NUMRL2) AFTER NUMRL2
C                       HAS BEEN INCREASED BY ONE.
C
C           SMALL     - LENGTH OF THE SMALLEST INTERVAL CONSIDERED
C                       UP TO NOW, MULTIPLIED BY 1.5
C
C           ERLARG    - SUM OF THE ERRORS OVER THE INTERVALS LARGER
C                       THAN THE SMALLEST INTERVAL
C                       CONSIDERED UP TO NOW
C           EXTRAP    - LOGICAL VARIABLE DENOTING THAT THE
C                       ROUTINE IS ATTEMPTING TO PERFORM
C                       EXTRAPOLATION.  I.E. BEFORE
C                       SUBDIVIDING THE SMALLEST INTERVAL
C                       WE TRY TO DECREASE THE VALUE OF
C                       ERLARG
C           NOEXT     - LOGICAL VARIABLE DENOTING THAT EXTRAPOLATION
C                       IS NO LONGER ALLOWED(/TRUE/ VALUE)
C
C           FIRST APPROXIMATION TO THE INTEGRAL
C           -----------------------------------
C
      LAST1 = 1
      IER = 0
      IERRO = 0
      CALL D01AJZ(F, A, B, RESULT, ABSERR, DEFABS, RESABS)
C
C           TEST ON ACCURACY
C
      DRES = ABS(RESULT)
      ERRBND = AMAX1(EPSABS,EPSREL*DRES)
      IF (ABSERR.LE.1.0E+02*EPMACH*DEFABS .AND. ABSERR.GT.ERRBND)
     * IER = 2
      IF (LIMIT.LT.2 .AND. ABSERR.GT.ERRBND) IER = 1
      IF (IER.NE.0 .OR. ABSERR.LE.ERRBND) GO TO 320
C
C           INITIALIZATION
C           --------------
C
      ALIST(1) = A
      BLIST(1) = B
      RLIST(1) = RESULT
      RLIST2(1) = RESULT
      ERRMAX = ABSERR
      MAXERR = 1
      AREA = RESULT
      ERRSUM = ABSERR
      ABSERR = OFLOW
      NRMAX = 1
      NRES = 0
      NUMRL2 = 2
      KTMIN = 0
      EXTRAP = .FALSE.
      NOEXT = .FALSE.
      IROFF1 = 0
      IROFF2 = 0
      IROFF3 = 0
      KSGN = -1
      IF (DRES.GE.(0.1E+01-0.5E+02*EPMACH)*DEFABS) KSGN = 1
C
C           MAIN DO-LOOP
C           ------------
C
      IF (LIMIT.LT.2) GO TO 220
      DO 200 LAST=2,LIMIT
C
C           BISECT THE SUBINTERVAL WITH THE NRMAX-TH LARGEST
C           ERROR ESTIMATE
C
         LAST1 = LAST
         A1 = ALIST(MAXERR)
         B1 = 0.5E+00*(ALIST(MAXERR)+BLIST(MAXERR))
         A2 = B1
         B2 = BLIST(MAXERR)
         ERLAST = ERRMAX
         CALL D01AJZ(F, A1, B1, AREA1, ERROR1, RESABS, DEFAB1)
         CALL D01AJZ(F, A2, B2, AREA2, ERROR2, RESABS, DEFAB2)
C
C           IMPROVE PREVIOUS APPROXIMATION OF INTEGRAL
C           AND ERROR AND TEST FOR ACCURACY
C
         AREA12 = AREA1 + AREA2
         ERRO12 = ERROR1 + ERROR2
         ERRSUM = ERRSUM + ERRO12 - ERRMAX
         AREA = AREA + AREA12 - RLIST(MAXERR)
         IF (DEFAB1.EQ.ERROR1 .OR. DEFAB2.EQ.ERROR2) GO TO 40
         IF (ABS(RLIST(MAXERR)-AREA12).GT.0.1E-04*ABS(AREA12) .OR.
     *    ERRO12.LT.0.99E+00*ERRMAX) GO TO 20
         IF (EXTRAP) IROFF2 = IROFF2 + 1
         IF (.NOT.EXTRAP) IROFF1 = IROFF1 + 1
   20    IF (LAST.GT.10 .AND. ERRO12.GT.ERRMAX) IROFF3 = IROFF3 + 1
   40    RLIST(MAXERR) = AREA1
         RLIST(LAST) = AREA2
         ERRBND = AMAX1(EPSABS,EPSREL*ABS(AREA))
         IF (ERRSUM.LE.ERRBND) GO TO 280
C
C           TEST FOR ROUNDOFF ERROR AND EVENTUALLY
C           SET ERROR FLAG
C
```

```
      IF (IROFF1+IROFF2.GE.10 .OR. IROFF3.GE.20) IER = 2
      IF (IROFF2.GE.5) IERRO = 3
C
C           SET ERROR FLAG IN THE CASE THAT THE NUMBER OF INTERVAL
C            BISECTIONS EXCEEDS /LIMIT/
C
      IF (LAST.EQ.LIMIT) IER = 1
C
C           SET ERROR FLAG IN THE CASE OF BAD INTEGRAND BEHAVIOUR
C           AT INTERIOR POINTS OF INTEGRATION RANGE
C
      IF (AMAX1(ABS(A1),ABS(B2)).LE.(0.1E+01+0.1E+03*EPMACH)*
     *  (ABS(A2)+0.1E+04*UFLOW)) IER = 4
      IF (IER.NE.0) GO TO 220
C
C           APPEND THE NEWLY-CREATED INTERVALS TO THE LIST
C
      IF (ERROR2.GT.ERROR1) GO TO 60
      ALIST(LAST) = A2
      BLIST(MAXERR) = B1
      BLIST(LAST) = B2
      ELIST(MAXERR) = ERROR1
      ELIST(LAST) = ERROR2
      GO TO 80
   60 ALIST(MAXERR) = A2
      ALIST(LAST) = A1
      BLIST(LAST) = B1
      RLIST(MAXERR) = AREA2
      RLIST(LAST) = AREA1
      ELIST(MAXERR) = ERROR2
      ELIST(LAST) = ERROR1
C
C           CALL SUBROUTINE D01AJX TO MAINTAIN THE
C           DESCENDING ORDERING IN THE LIST OF ERROR
C           ESTIMATES AND SELECT THE SUBINTERVAL WITH
C           NRMAX-TH LARGEST ERROR ESTIMATE (TO BE BISECTED
C           NEXT)
C
   80 CALL D01AJX(LIMIT, LAST, MAXERR, ERRMAX, ELIST, IORD,
     *  LIORD, NRMAX)
      IF (LAST.EQ.2) GO TO 180
      IF (NOEXT) GO TO 200
      ERLARG = ERLARG - ERLAST
      IF (ABS(B1-A1).GT.SMALL) ERLARG = ERLARG + ERRO12
      IF (EXTRAP) GO TO 100
C
C           TEST WHETHER THE INTERVAL TO BE BISECTED NEXT IS THE
C           SMALLEST INTERVAL
C
      IF (ABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200
      EXTRAP = .TRUE.
      NRMAX = 2
  100 IF (IERRO.EQ.3 .OR. ERLARG.LE.ERTEST) GO TO 140
C
C           THE SMALLEST INTERVAL HAS THE LARGEST ERROR.
C           BEFORE BISECTING DECREASE THE SUM OF THE ERRORS
```

```
C               OVER THE LARGER INTERVALS(ERLARG) AND PERFORM
C               EXTRAPOLATION
C
            ID = NRMAX
            DO 120 K=ID,JUPBND
               MAXERR = IORD(NRMAX)
               ERRMAX = ELIST(MAXERR)
               IF (ABS(BLIST(MAXERR)-ALIST(MAXERR)).GT.SMALL) GO TO 200
               NRMAX = NRMAX + 1
  120       CONTINUE
C
C              PERFORM EXTRAPOLATION
C
  140       NUMRL2 = NUMRL2 + 1
            RLIST2(NUMRL2) = AREA
            CALL D01AJY(NUMRL2, RLIST2, RESEPS, ABSEPS, RES3LA, NRES)
            KTMIN = KTMIN + 1
            IF (KTMIN.GT.5 .AND. ABSERR.LT.0.1E-02*ERRSUM) IER = 5
            IF (ABSEPS.GE.ABSERR) GO TO 160
            KTMIN = 0
            ABSERR = ABSEPS
            RESULT = RESEPS
            CORREC = ERLARG
            ERTEST = AMAX1(EPSABS,EPSREL*ABS(RESEPS))
            IF (ABSERR.LE.ERTEST) GO TO 220
C
C              PREPARE  BISECTION OF THE SMALLEST INTERVAL
C
  160       IF (NUMRL2.EQ.1) NOEXT = .TRUE.
            IF (IER.EQ.5) GO TO 220
            MAXERR = IORD(1)
            ERRMAX = ELIST(MAXERR)
            NRMAX = 1
            EXTRAP = .FALSE.
            SMALL = SMALL*0.5E+00
            ERLARG = ERRSUM
            GO TO 200
  180       SMALL = ABS(B-A)*0.375E+00
            ERLARG = ERRSUM
            ERTEST = ERRBND
            RLIST2(2) = AREA
  200 CONTINUE
C
C              SET  FINAL RESULT AND ERROR ESTIMATE
C              ------------------------------------
C
  220 IF (ABSERR.EQ.OFLOW) GO TO 280
      IF (IER+IERRO.EQ.0) GO TO 260
      IF (IERRO.EQ.3) ABSERR = ABSERR + CORREC
      IF (IER.EQ.0) IER = 3
      IF (RESULT.NE.0.E+00.AND .AREA. NE.0.E+00) GO TO 240
      IF (ABSERR.GT.ERRSUM) GO TO 280
      IF (AREA.EQ.0.E+00) GO TO 320
      GO TO 260
  240 IF (ABSERR/ABS(RESULT).GT.ERRSUM/ABS(AREA)) GO TO 280
C
```

```
C           TEST ON DIVERGENCY
C
  260 IF (KSGN.EQ.-1 .AND. AMAX1(ABS(RESULT),ABS(AREA)).LE.DEFABS*
     * 0.1E-01) GO TO 320
      IF (0.1E-01.GT.(RESULT/AREA) .OR. (RESULT/AREA).GT.0.1E+03
     * .OR. ERRSUM.GT.ABS(AREA)) IER = 6
      GO TO 320
C
C           COMPUTE GLOBAL INTEGRAL SUM
C
  280 RESULT = 0.E+00
      DO 300 K=1,LAST
         RESULT = RESULT + RLIST(K)
  300 CONTINUE
      ABSERR = ERRSUM
  320 IF (IER.GT.2) IER = IER - 1
      IORD(1) = 4*LAST1
      RETURN
      END
      SUBROUTINE D01AJX(LIMIT, LAST, MAXERR, ERMAX, ELIST, IORD,
     * LIORD, NRMAX)
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE ORDER
C     **************************************************************
C
C           PURPOSE
C              THIS ROUTINE MAINTAINS THE DESCENDING ORDERING
C              IN THE LIST OF THE LOCAL ERROR ESTIMATES
C              RESULTING FROM THE INTERVAL SUBDIVISION
C              PROCESS. AT EACH CALL TWO ERROR ESTIMATES
C              ARE INSERTED USING THE SEQUENTIAL SEARCH
C              METHOD . TOP-DOWN FOR THE LARGEST ERROR
C              ESTIMATE,  BOTTOM-UP FOR THE SMALLEST ERROR
C              ESTIMATE.
C
C           CALLING SEQUENCE
C              CALL D01AJX
C              (LIMIT,LAST,MAXERR,ERMAX,ELIST,IORD,LIORD,NRMAX)
C
C             PARAMETERS (MEANING AT OUTPUT)
C              LIMIT  - MAXIMUM NUMBER OF ERROR ESTIMATES THE LIST
C                       CAN CONTAIN
C
C              LAST   - NUMBER OF ERROR ESTIMATES CURRENTLY
C                       IN THE LIST. ELIST(LAST) CONTAINS
C                       THE SMALLEST ERROR ESTIMATE.
C
C              MAXERR - MAXERR POINTS TO THE NRMAX-TH LARGEST ERROR
C                       ESTIMATE CURRENTLY IN THE LIST.
C
C              ERMAX  - NRMAX-TH LARGEST ERROR ESTIMATE
C                       ERMAX = ELIST(MAXERR)
C
C              ELIST  - ARRAY OF DIMENSION LAST CONTAINING
C                       THE ERROR ESTIMATES
C
```

```
C             IORD   - ARRAY CONTAINING POINTERS TO ELIST SO
C                      THAT IORD(1) POINTS TO THE LARGEST
C                      ERROR ESTIMATE,...,IORD(LAST) TO THE
C                      SMALLEST ERROR ESTIMATE
C
C             LIORD  - DIMENSION OF IORD
C
C             NRMAX  - MAXERR = IORD(NRMAX)
C
C     ******************************************************
C
C     .. SCALAR ARGUMENTS ..
      REAL ERMAX
      INTEGER LAST, LIMIT, LIORD, MAXERR, NRMAX
C     .. ARRAY ARGUMENTS ..
      REAL ELIST(LAST)
      INTEGER IORD(LIORD)
C     ..
C     .. SCALARS IN COMMON ..
      INTEGER JUPBND
C     ..
C     .. LOCAL SCALARS ..
      REAL ERRMAX, ERRMIN
      INTEGER I, IBEG, IDO, ISUCC, J, JBND, K
C     ..
      COMMON /AD01AJ/ JUPBND
C
C            CHECK WHETHER THE LIST CONTAINS MORE THAN
C            TWO ERROR ESTIMATES
C
      IF (LAST.GT.2) GO TO 20
      IORD(1) = 1
      IORD(2) = 2
      GO TO 100
C
C           THIS PART OF THE ROUTINE IS ONLY EXECUTED
C           IF, DUE TO A DIFFICULT INTEGRAND, SUBDIVISION
C           INCREASED THE ERROR ESTIMATE. IN THE NORMAL CASE
C           THE INSERT PROCEDURE SHOULD START AFTER THE
C           NRMAX-TH LARGEST ERROR ESTIMATE.
C
   20 ERRMAX = ELIST(MAXERR)
      IF (NRMAX.EQ.1) GO TO 60
      IDO = NRMAX - 1
      DO 40 I=1,IDO
         ISUCC = IORD(NRMAX-1)
         IF (ERRMAX.LE.ELIST(ISUCC)) GO TO 60
         IORD(NRMAX) = ISUCC
         NRMAX = NRMAX - 1
   40 CONTINUE
C
C           COMPUTE THE NUMBER OF ELEMENTS IN THE LIST TO
C           BE MAINTAINED IN DESCENDING ORDER. THIS NUMBER
C           DEPENDS ON THE NUMBER OF SUBDIVISIONS STILL
C           ALLOWED
C
```

```
   60 JUPBND = LAST
      IF (LAST.GT.(LIMIT/2+2)) JUPBND = LIMIT + 3 - LAST
      ERRMIN = ELIST(LAST)
C
C           INSERT ERRMAX BY TRAVERSING THE LIST TOP-DOWN
C           STARTING COMPARISON FROM THE ELEMENT
C           ELIST(IORD(NRMAX+1))
C
      JBND = JUPBND - 1
      IBEG = NRMAX + 1
      IF (IBEG.GT.JBND) GO TO 100
      DO 80 I=IBEG,JBND
         ISUCC = IORD(I)
         IF (ERRMAX.GE.ELIST(ISUCC)) GO TO 120
         IORD(I-1) = ISUCC
   80 CONTINUE
  100 IORD(JBND) = MAXERR
      IORD(JUPBND) = LAST
      GO TO 180
C
C           INSERT ERRMIN BY TRAVERSING THE LIST BOTTOM-UP
C
  120 IORD(I-1) = MAXERR
      K = JBND
      DO 140 J=I,JBND
         ISUCC = IORD(K)
         IF (ERRMIN.LT.ELIST(ISUCC)) GO TO 160
         IORD(K+1) = ISUCC
         K = K - 1
  140 CONTINUE
      IORD(I) = LAST
      GO TO 180
  160 IORD(K+1) = LAST
C
C           SET MAXERR AND ERMAX
C
  180 MAXERR = IORD(NRMAX)
      ERMAX = ELIST(MAXERR)
      RETURN
      END
      SUBROUTINE D01AJY(N, EPSTAB, RESULT, ABSERR, RES3LA, NRES)
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE EPSALG
C     **********************************************************
C
C           PURPOSE
C              THE ROUTINE TRANSFORMS A GIVEN SEQUENCE OF
C              APPROXIMATIONS, BY MEANS OF THE EPSILON
C              ALGORITHM OF P. WYNN.
C
C              AN ESTIMATE OF THE ABSOLUTE ERROR IS ALSO GIVEN.
C              THE CONDENSED EPSILON TABLE IS COMPUTED. ONLY THOSE
C              ELEMENTS NEEDED FOR THE COMPUTATION OF THE
C              NEXT DIAGONAL ARE PRESERVED.
C
C           CALLING SEQUENCE
```

```
C           CALL D01AJY (N,EPSTAB,RESULT,ABSERR,RES3LA,NRES)
C
C        PARAMETERS
C           N      - EPSTAB(N) CONTAINS THE NEW ELEMENT IN THE
C                    FIRST COLUMN OF THE EPSILON TABLE.
C
C           EPSTAB - ONE DIMENSIONAL ARRAY CONTAINING THE
C                    ELEMENTS OF THE TWO LOWER DIAGONALS OF
C                    THE TRIANGULAR EPSILON TABLE.
C                    THE ELEMENTS ARE NUMBERED STARTING AT THE
C                    RIGHT-HAND CORNER OF THE TRIANGLE.
C                    THE DIMENSION SHOULD BE AT LEAST N+2.
C
C           RESULT - RESULTING APPROXIMATION TO THE INTEGRAL
C
C           ABSERR - ESTIMATE OF THE ABSOLUTE ERROR COMPUTED FROM
C                    RESULT AND THE 3 PREVIOUS /RESULTS/
C
C           RES3LA - ARRAY CONTAINING THE LAST 3 /RESULTS/
C
C           NRES   - NUMBER OF CALLS TO THE ROUTINE
C                    (SHOULD BE ZERO AT FIRST CALL)
C
C     ******************************************************
C     ..SCALAR ARGUMENTS ..
      REL ABSERR, RESULT
      INEGER N, NRES
C     ..ARRAY ARGUMENTS ..
      REL EPSTAB(52), RES3LA(3)
C     ..
C     ..LOCAL SCALARS ..
      REL DELTA1, DELTA2, DELTA3, E0, E1, E1ABS, E2, E3, EPMACH,
     * ESINF, ERR1, ERR2, ERR3, ERROR, OFLOW, RES, SS, TOL1, TOL2,
     * TL3
      INEGER I, IB2, IB, IE, IND, K1, K2, K3, LIMEXP, NEWELM, NUM
C     ..FUNCTION REFERENCES ..
      REL X02AAF, X02ACF
C     ..
C
C            MACHINE DEPENDENT CONSTANTS
C             -------------------------
C            /LIMEXP/ IS THE MAXIMUM NUMBER OF ELEMENTS THE EPSILON
C            TABLE CAN CONTAIN. IF THIS NUMBER IS REACHED, THE UPPER
C            DIAGONAL OF THE EPSILON TABLE IS DELETED.
C
      DA LIMEXP /50/
      EPACH = X02AAF(1.0)
      OFOW = X02ACF(1.0)
C
C           LIST OF MAJOR VARIABLES
C           -----------------------
C           E0     - THE 4 ELEMENTS ON WHICH THE
C           E1       COMPUTATION OF A NEW ELEMENT IN
C           E2       THE EPSILON TABLE IS BASED
C           E3                 E0
C                        E3    E1    NEW
```

```
C                           E2
C          NEWELM - NUMBER OF ELEMENTS TO BE COMPUTED IN THE NEW
C                   DIAGONAL
C          ERROR  - ERROR = ABS(E1-E0)+ABS(E2-E1)+ABS(NEW-E2)
C          RESULT - THE ELEMENT IN THE NEW DIAGONAL WITH LEAST
C                   ERROR
C
      NRES = NRES + 1
      ABSERR = OFLOW
      RESULT = EPSTAB(N)
      IF (N.LT.3) GO TO 200
      EPSTAB(N+2) = EPSTAB(N)
      NEWELM = (N-1)/2
      EPSTAB(N) = OFLOW
      NUM = N
      K1 = N
      DO 80 I=1,NEWELM
         K2 = K1 - 1
         K3 = K1 - 2
         RES = EPSTAB(K1+2)
         E0 = EPSTAB(K3)
         E1 = EPSTAB(K2)
         E2 = RES
         E1ABS = ABS(E1)
         DELTA2 = E2 - E1
         ERR2 = ABS(DELTA2)
         TOL2 = AMAX1(ABS(E2),E1ABS)*EPMACH
         DELTA3 = E1 - E0
         ERR3 = ABS(DELTA3)
         TOL3 = AMAX1(E1ABS,ABS(E0))*EPMACH
         IF (ERR2.GT.TOL2 .OR. ERR3.GT.TOL3) GO TO 20
C
C           IF E0, E1 AND E2 ARE EQUAL TO WITHIN MACHINE
C           ACCURACY, CONVERGENCE IS ASSUMED
C           RESULT = E2
C           ABSERR = ABS(E1-E0)+ABS(E2-E1)
C
         RESULT = RES
         ABSERR = ERR2 + ERR3
         GO TO 200
   20    E3 = EPSTAB(K1)
         EPSTAB(K1) = E1
         DELTA1 = E1 - E3
         ERR1 = ABS(DELTA1)
         TOL1 = AMAX1(E1ABS,ABS(E3))*EPMACH
C
C           IF TWO ELEMENTS ARE VERY CLOSE TO EACH OTHER, OMIT
C           A PART OF THE TABLE BY ADJUSTING THE VALUE OF N
C
         IF (ERR1.LT.TOL1 .OR. ERR2.LT.TOL2 .OR. ERR3.LT.TOL3) GO
     *    TO 40
         SS = 0.1E+01/DELTA1 + 0.1E+01/DELTA2 - 0.1E+01/DELTA3
         EPSINF = ABS(SS*E1)
C
C           TEST TO DETECT IRREGULAR BEHAVIOUR IN THE TABLE, AND
C           EVENTUALLY OMIT A PART OF THE TABLE ADJUSTING THE VALUE
```

```
C           OF N
C
         IF (EPSINF.GT.0.1E-03) GO TO 60
   40    N = I + I - 1
         GO TO 100
C
C           COMPUTE A NEW ELEMENT AND EVENTUALLY ADJUST
C           THE VALUE OF RESULT
C
   60    RES = E1 + 0.1E+01/SS
         EPSTAB(K1) = RES
         K1 = K1 - 2
         ERROR = ERR2 + ABS(RES-E2) + ERR3
         IF (ERROR.GT.ABSERR) GO TO 80
         ABSERR = ERROR
         RESULT = RES
   80 CONTINUE
C
C           SHIFT THE TABLE
C
  100 IF (N.EQ.LIMEXP) N = 2*(LIMEXP/2) - 1
      IB = 1
      IF ((NUM/2)*2.EQ.NUM) IB = 2
      IE = NEWELM + 1
      DO 120 I=1,IE
         IB2 = IB + 2
         EPSTAB(IB) = EPSTAB(IB2)
         IB = IB2
  120 CONTINUE
      IF (NUM.EQ.N) GO TO 160
      IND = NUM - N + 1
      DO 140 I=1,N
         EPSTAB(I) = EPSTAB(IND)
         IND = IND + 1
  140 CONTINUE
  160 IF (NRES.GE.4) GO TO 180
      RES3LA(NRES) = RESULT
      ABSERR = OFLOW
      GO TO 200
C
C           COMPUTE ERROR ESTIMATE
C
  180 ABSERR = ABS(RESULT-RES3LA(3)) + ABS(RESULT-RES3LA(2)) +
     * ABS(RESULT-RES3LA(1))
      RES3LA(1) = RES3LA(2)
      RES3LA(2) = RES3LA(3)
      RES3LA(3) = RESULT
  200 ABSERR = AMAX1(ABSERR,5.0E+00*EPMACH*ABS(RESULT))
      RETURN
      END
      SUBROUTINE D01AJE(F, A, B, RESULT, ABSERR, RESABS, RESASC)
C     MARK 8 RELEASE. NAG COPYRIGHT 1979
C     BASED ON QUADPACK ROUTINE QUAGS
C     **************************************************
C
C           PURPOSE
```

```
C            TO COMPUTE I = INTEGRAL OF F OVER (A,B), WITH ERROR
C                           ESTIMATE
C       J = INTEGRAL OF ABS(F) OVER (A,B)
C
C          CALLING SEQUENCE
C             CALL D01AJZ (F,A,B,RESULT,ABSERR,RESABS,RESASC)
C
C          PARAMETERS
C             F      - FUNCTION SUBPROGRAM DEFINING THE INTEGRAND
C                      FUNCTION F(X). THE ACTUAL NAME FOR F NEEDS
C                      TO BE DECLARED E X T E R N A L IN THE
C                      CALLING PROGRAM
C
C             A      - LOWER LIMIT OF INTEGRATION
C
C             B      - UPPER LIMIT OF INTEGRATION
C
C             RESULT - APPROXIMATION TO THE INTEGRAL I.
C                      RESULT IS CALCULATED BY APPLYING
C                      THE 21-POINT GAUSS-KRONROD RULE
C                      (RESK), OBTAINED BY OPTIMAL
C                      ADDITION OF ABSCISSAE TO THE
C                      10-POINT GAUSS  RULE (RESG).
C
C             ABSERR - ESTIMATE OF THE MODULUS OF THE
C                      ABSOLUTE ERROR, WHICH SHOULD NOT
C                      EXCEED ABS(I-RESULT)
C             RESABS - APPROXIMATION TO THE INTEGRAL J
C
C             RESASC - APPROXIMATION TO THE INTEGRAL OF
C                      ABS(F-I/(B-A)) OVER (A,B)
C
C     ***********************************************************
C     .. SCALAR ARGUMENTS ..
      REAL A, ABSERR, B, RESABS, RESASC, RESULT
C     .. FUNCTION ARGUMENTS ..
      REAL F
C     ..
C     .. LOCAL SCALARS ..
      REAL ABSC, CENTRE, DHLGTH, EPMACH, FC, FSUM, FVAL1, FVA2,
     * HLGTH, RESG, RESK, RESKH, UFLOW
      INTEGER J
C     .. LOCAL ARRAYS ..
      REAL FV1(10), FV2(10), WG(10), WGK(11), XGK(11)
C     .. FUNCTION REFERENCES ..
      REAL X02AAF, X02ABF
C     ..
C
C             THE ABSCISSAE AND WEIGHTS ARE GIVEN FOR THE
C             INTERVAL (-1,1) . BECAUSE OF SYMMETRY ONLY THE
C             POSITIVE ABSCISSAE AND THEIR CORRESPONDING
C             WEIGHTS ARE GIVEN.
C             XGK    - ABSCISSAE OF THE 21-POINT GAUSS-KRONRODRULE
C                      XGK(2), XGK(4), ..... ABSCISSAE OF THE 1-POINT
C                      GAUSS RULE
C                      XGK(1), XGK(3), ..... ABSCISSAE WHICH
```

```
C                    ARE OPTIMALLY ADDED TO THE 10-POINT
C                    GAUSS RULE
C           WGK    - WEIGHTS OF THE 21-POINT GAUSS-KRONROD RULE
C           WG     - WEIGHTS OF THE 10-POINT GAUSS RULE,
C                    CORRESPONDING TO THE ABSCISSAE XGK(2),
C                    XGK(4), ... WG(1), WG(3), ... ARE SET
C                    TO ZERO.
C
      DATA XGK(1), XGK(2), XGK(3), XGK(4), XGK(5), XGK(6), XGK(7),
     * XGK(8), XGK(9), XGK(10), XGK(11) /0.995657163025808080735527
     * 807E+00,0.973906528517171720077964012 1E+00,
     * 0.930157491355708226001207180 1E+00,0.865063366688984510732096
     * 6884E+00,0.780817726586416897063717578 3E+00,
     * 0.679409568299024406234327365 1E+00,0.562757134668604683339000
     * 0993E+00,0.433395394129247190799265943 2E+00,
     * 0.294392862701460198131126603 1E+00,0.148874338981631210884826
     * 0011E+00,0.0/
      DATA WGK(1), WGK(2), WGK(3), WGK(4), WGK(5), WGK(6), WGK(7),
     * WGK(8), WGK(9), WGK(10), WGK(11) /0.116946388673718742780643
     * 9606E-01,0.325581623079647274788189724 6E-01,
     * 0.547558965743519960313813002 4E-01,0.750396748109199527670431
     * 4092E-01,0.931254545836976055350654650 8E-01,
     * 0.109387158802297641899210590 3E+00,0.123491976262065851077958
     * 1098E+00,0.134709217311473325928054001 8E+00,
     * 0.142775938577060080797094273 1E+00,0.147739104901338491374841
     * 5160E+00,0.149445554002916905664936468 4E+00/
      DATA WG(1), WG(2), WG(3), WG(4), WG(5), WG(6), WG(7), WG(8),
     * WG(9), WG(10) /0.0,0.666713443086881375935688098 9E-01,0.0,
     * 0.149451349150580593145776339 7E+00,0.0,0.219086362515982043995
     * 5349342E+00,0.0,0.269266719309996355091226921 6E+00,0.0,
     * 0.295524224714752870173892994 7E+00/
      EPMACH = X02AAF(1.0)
      UFLOW = X02ABF(1.0)
C
C           LIST OF MAJOR VARIABLES
C           ----------------------
C           CENTRE - MID POINT OF THE INTERVAL
C           HLGTH  - HALF LENGTH OF THE INTERVAL
C           ABSC   - ABSCISSA
C           FVAL*  - FUNCTION VALUE
C           RESG   - 10-POINT GAUSS FORMULA
C           RESK   - 21-POINT GAUSS-KRONROD FORMULA
C           RESKH  - APPROXIMATION TO MEAN VALUE OF F OVER
C                    (A,B), I.E. TO I/(B-A)
C
      CENTRE = 0.5E+00*(A+B)
      HLGTH = 0.5E+00*(B-A)
      DHLGTH = ABS(HLGTH)
C
C           COMPUTE THE 21-POINT GAUSS-KRONROD APPROXIMATION TO
C           THE INTEGRAL, AND ESTIMATE THE ABSOLUTE ERROR
C
      RESG = 0.0E+00
      FC = F(CENTRE)
      RESK = WGK(11)*FC
      RESABS = ABS(RESK)
      DO 20 J=1,10
         ABSC = HLGTH*XGK(J)
         FVAL1 = F(CENTRE-ABSC)
         FVAL2 = F(CENTRE+ABSC)
         FV1(J) = FVAL1
         FV2(J) = FVAL2
         FSUM = FVAL1 + FVAL2
         RESG = RESG + WG(J)*FSUM
         RESK = RESK + WGK(J)*FSUM
         RESABS = RESABS + WGK(J)*(ABS(FVAL1)+ABS(FVAL2))
   20 CONTINUE
      RESKH = RESK*0.5E+00
      RESASC = WGK(11)*ABS(FC-RESKH)
      DO 40 J=1,10
         RESASC = RESASC + WGK(J)*(ABS(FV1(J)-RESKH)+ABS(FV2(J)
     *    -RESKH))
   40 CONTINUE
      RESULT = RESK*HLGTH
      RESABS = RESABS*DHLGTH
      RESASC = RESASC*DHLGTH
      ABSERR = ABS((RESK-RESG)*HLGTH)
      IF (RESASC.NE.0.E+00) ABSERR = RESASC*AMIN1(0.1E+01,(0.2E+03*
     * ABSERR/RESASC)**1.5E0)
      IF (RESABS.GT.UFLOW/(0.5E+02*EPMACH)) ABSERR =
     * AMAX1(EPMACH*RESABS*0.5E+02,ABSERR)
      RETURN
      END
      INTEGER FUNCTION P01AAF(IFAIL, ERROR, SRNAME)
C     MARK 1 RELEASE.  NAG COPYRIGHT 1971
C     MARK 3 REVISED
C     MARK 4A REVISED, IER-45
C     MARK 4.5 REVISED
C     MARK 7 REVISED (DEC 1978) .... (APR 1979)
C     RETURNS THE VALUE OF ERROR OR TERMINATES THE PROGRAM.
C     IF A HARD FAILURE OCCURS, THIS ROUTINE CALLS A FORTRAN AUXILIARY
C     ROUTINE P01AAZ WHICH GIVES A TRACE, A FAILURE MESSAGE AND HALTS
C     THE PROGRAM
      INTEGER ERROR, IFAIL, NOUT
      DOUBLE PRECISION SRNAME
C     TEST IF NO ERROR DETECTED
      IF (ERROR.EQ.0) GO TO 20
C     DETERMINE OUTPUT UNIT FOR MESSAGE
      CALL X04AAF (0,NOUT)
C     TEST FOR SOFT FAILURE
      IF (MOD(IFAIL,10).EQ.1) GO TO 10
C     HARD FAILURE
      WRITE (NOUT,99999) SRNAME, ERROR
C     STOPPING MECHANISM MAY ALSO DIFFER
      CALL P01AAZ (X)
C     STOP
C     SOFT FAIL
C     TEST IF ERROR MESSAGES SUPPRESSED
   10 IF (MOD(IFAIL/10,10).EQ.0) GO TO 20
      WRITE (NOUT,99999) SRNAME, ERROR
   20 P01AAF = ERROR
      RETURN
```

```
99999 FORMAT (1H0, 38HERROR DETECTED BY NAG LIBRARY ROUTINE , A8,
     * 11H - IFAIL = , I5//)
      END
      SUBROUTINE P01AAZ
C    MARK 2 RELEASE. TOM THACKER AND JOYCE CLARKE  OEG OXFORD
C    MARK 6 REVISED.
C     CALL TRACE
      STOP
      END
C     AUTO EDIT 20 SEP 76
      REAL FUNCTION X02AAF(X)
C     NAG COPYRIGHT 1975
C     EDITED BY JOYCE CLARKE OXFORD OEG NUCLEAR PHYSICS 03RD OCT 1976
C                  FORTRAN MACRO VERSION FDIA26.TEC
C     MARK 4.5 RELEASE

C     * EPS *
C     RETURNS THE VALUE EPS WHERE EPS IS THE SMALLEST
C     POSITIVE
C     NUMBER SUCH THAT 1.0 + EPS > 1.0
C     THE X PARAMETER IS NOT USED
C     FOR ICL 1900
C     X02AAF = 2.0**(-37.0)
      REAL X
      X02AAF = 9.54E-7
C     X02AAF = "146400000000
      RETURN
      END
C     AUTO EDIT 17 OCT 76
      REAL FUNCTION X02ABF(X)
C     NAG COPYRIGHT 1975
C     EDITED BY JOYCE CLARKE OXFORD OEG NUCLEAR PHYSICS 03RD OCT 1976
C                  FORTRAN MACRO VERSION FDIA26.TEC
C     MARK 4.5 RELEASE

C     * RMIN *
C     RETURNS THE VALUE OF THE SMALLEST POSITIVE REAL FLOATING-
C     POINT NUMBER EXACTLY REPRESENTABLE ON THE COMPUTER
C     THE X PARAMETER IS NOT USED
C     FOR ICL 1900
C     X02ABF = 2.0**(-257.0)
      REAL X
C     X02ABF = "000400000000
      X02ABF = 5.4E-79
      RETURN
      END
C     AUTO EDIT 17 OCT 76 -
      REAL FUNCTION X02ACF(X)
C     NAG COPYRIGHT 1975
C     EDITED BY JOYCE CLARKE OXFORD OEG NUCLEAR PHYSICS 03RD OCT 1976
C                  FORTRAN MACRO VERSION FDIA26.TEC
C     MARK 4.5 RELEASE

C     * RMAX *
C     RETURNS THE VALUE OF THE LARGEST POSITIVE REAL  FLOATING-
C     POINT NUMBER REPRESENTABLE ON THE COMPUTER
```

```
C      FOR ICL 1900
C      X02ACF = (2.0 - 2.0**(-36.0))*2.0**254.0
       REAL X
C      X02ACF = "377777777777
       X02ACF = 7.24E+75
       RETURN
       END
       SUBROUTINE X04AAF(I,NERR)
C      MARK 7 RELEASE. NAG COPYRIGHT 1978
C      EDITED BY JOYCE CLARKE OXFORD OEG NUCLEAR PHYSICS 05TH NOV 1976
C                   FORTRAN MACRO VERSION FDIA26.TEC
C      IF I = 0, SETS NERR TO CURRENT ERROR MESSAGE UNIT NUMBER
C      (STORED IN NERR1).
C      IF I = 1, CHANGES CURRENT ERROR MESSAGE UNIT NUMBER TO
C      VALUE SPECIFIED BY NERR.
C
C      ***NOTE ***
C      THI  ROUTINE ASSUMES THAT THE VALUE OF NERR1 IS SAVED
C      BETEEN CALLS.  IN SOME IMPLEMENTATIONS IT MAY BE
C      NECSSARY TO STORE NERR1 IN A LABELLED COMMON
C      BLOK /AX02AA/ TO ACHIEVE THIS.
C                                                                52000000
C      .. SCALAR ARGUMENTS ..
       INTGER I, NERR
C      ..
C      .. LOCAL SCALARS ..
       INTGER NERR1
C      ..
       DAT NERR1 /-1/
       IF I.EQ.0) NERR = NERR1
       IF I.EQ.1) NERR1 = NERR
       RETRN
       END
```

APPENDIX F

DESCRIPTION OF METHODS USED TO ESTIMATE BIOACCUMULATION IN FOOD CHAINS

In order to assess human exposure to chemicals present in air, water, and soil, it is necessary to estimate bioaccumulation in food animals or crops comprising the human diet. However, the subject of bioaccumulation was not a part of the original scope of the TOX-SCREEN model, and thus was not addressed in the initial model documentation (McDowell-Boyer and Hetrick, 1982). This appendix is to serve as a description of preliminary methods adopted to estimate bioaccumulation in aquatic organisms, food animals, and plants in TOX-SCREEN. An in-depth analysis of pertinent literature, however, was not possible due to time constraints.

Bioaccumulation in aquatic organisms (as a group) is handled according to a regression line derived by Mackay (1982), which provides a correlation between the bioaccumulation factor, BCF (aq), and the octanol-water partition coefficient, K_{ow}. The line is represented by the equation

$$\text{BCF (aq)} = 0.048\ K_{ow},$$

where BCF (aq) is defined as the ratio between the concentration of a compound in the aquatic organism (μg/g fresh weight) and the concentration in water (μg/ml). This definition of BCF (aq) necessitates the assumption that the organism's fresh-weight density may be approximated as 1 g/cm^3.

A number of limitations are associated with this method, according to both Trabalka (1982) and Mackay (1982). First and foremost, bioaccumulation of a covalently bonding chemical cannot be predicted by this method. Second, size and steric properties of a compound may affect the degree of bioaccumulation, although the above regression equation considers only lipophilic properties. Furthermore, biodegradability of the compound by the organisms' enzymes may alter the BCF (aq) from that predicted by the regression equation. Also, equilibrium measurement of K_{ow} in excess of 10^6 is difficult, such that the BCF-K_{ow} correlation derived may fail for high-K_{ow} compounds (Mackay, 1982). The above equation considers only the chemical taken up directly from the water (bioconcentration); it does not consider the possibility of accumulation through the food chain (biomagnification), which may be the dominant route of uptake for chemicals with high log K_{ow}. Compounds with K_{ow}'s below 10 are also suspect with respect to BCF predictability. Finally, the BCF is sensitive to the lipid content of individual organisms, such that much variability is associated with a predicted BCF on this basis.

It is necessary in TOX-SCREEN to specify if a compound has a propensity for covalent bonding. If so, no concentrations in biota are calculated. If not, concentrations in aquatic organisms are calculated by

$$[\text{conc. in aquatic org.}] = \text{BCF (aq)} \times [\text{conc. in water}].$$

A reference to a footnote, which lists the limitations of the BCF-K_{ow} regression, is made when the calculated concentration is printed in the computer code output.

Bioaccumulation in terrestrial animals, more specifically, food animals such as cattle, will be handled in TOX-SCREEN in a somewhat more crude manner, due to the poorer correlation between BCF and K_{ow} than exists for aquatic organisms. A single numerical value of log K_{ow} is used to screen compounds with respect to their bioaccumulation potential in terrestrial animals, rather than a regression line, based on suggestions by Trabalka (1982). A log K_{ow} of 3.5 has been suggested as that value, which corresponds to a BCF (animal) of approximately 0.1 for mammals and birds. This value is used in the screening-level model to categorize compounds as either having BCF's greater than or less than 0.1. That is, if log K_{ow} is greater than or equal to 3.5, then a message is printed stating that the compound may be bioaccumulated with a BCF (animal) of at least 0.1. Otherwise (i.e., log K_{ow} is less than 3.5) a message is printed stating that the BCF (animal) is likely to be less than 0.1. Before this is done, however, it is again necessary to specify whether the compound forms covalent bonds and if so, the categorization according to K_{ow} is not performed. A reference to the footnote concerning limitations is again made in the output if categorization is performed.

The BCF (animal) is defined as the ratio of the compound's concentration in animal tissue to that in the animal's diet. Thus, if it were desirable to calculate the tissue concentration, it would be necessary to predict the dietary concentration. The TOX-SCREEN model provides concentrations in surface water, which may be a part of the animal's diet. However, in order to determine concentrations in foods and pasture, it is necessary to look at bioaccumulation in vegetation as a result of root uptake from soil and interception of depositing materials from air. In order to estimate root uptake of compounds, results of a recent ORNL study of the relationship between K_d (the soil-water partition coefficient) and BCF (plant) will be used in TOX-SCREEN (Baes, in press). The analysis of that relationship was done on an element-specific basis, rather than compound-specific, such that average K_d's and BCF's for each element were tabulated from a review of literature. Thus, the K_d's and BCF's are likely to be more variable within each element group than within a chemical compound group because of the variety of chemical forms that may have existed for each element for which parameters were measured. Regression analysis was done on paired elemental values, resulting in an expression of the form

$$\ln K_d = A + B\,[\ln \text{BCF (plant)}],$$

where A and B are parameters used to adjust the expression to fit the data. The values of A and B used in TOX-SCREEN are 3.02 and -0.85, respectively, which were derived from a literature review of 21 elements, although these values may vary considerably, depending on the methods of determining K_d (Baes, in press). The definition of BCF (plant) is the ratic of the mature plant parts concentration of a compound (μg/g dry weight) to the soil concentration (μg/g dry weight), so is unitless.

The value of K_d will be estimated in TOX-SCREEN with the relationship

$$K_d = K_{oc} \times \%oc,$$

where K_{oc} is the organic carbon sorption coefficient and %oc is the present organic carbon content of the soil. Both of these latter values are used in SESOIL, and so have already been input by the user before the bioaccumulation subroutine is called.

The concentration in plants as a result of root uptake of a compound is determined from

$$[\text{conc. in plants via roots}] = \text{BCF (plant)} \times [\text{conc. in soil}]$$

where concentrations are in µg per g dry weight. Because K_d is determined as a function of K_{oc}, and because a significant correlation between K_{oc} and K_{ow} has been noted by several investigators (Means et al., 1982; Karickhoff, 1979; Neely, 1981), the same limitations apply to this approach to estimating BCF (plant) as to the method for estimating BCF (aq), and notation as such is provided in the TOX-SCREEN output. Also, concentrations are not calculated for covalently bonding materials.

As was mentioned earlier, the concentration of a compound in plants may also be a result of interception of depositing material from the air. The interception model which is used in TOX-SCREEN was developed by Chamberlain (1971). This model also is similar to that provided in the U. S. Nuclear Regulatory Commission's Regulatory Guide 1.109 (USNRC,1977) for calculating vegetative concentrations as a result of nuclear reactor effluent releases. The concentration in plants (µg/g) due to interception is expressed by

[conc. in plants via interception] =

$$\frac{r}{Y_v \lambda_{Ei}} \left[1 - \frac{1 - e^{-\lambda_{Ei} t_e}}{\lambda_{Ei} t_e} \right] \times \text{[deposition rate]}$$

where r is an empirically determined initial interception fraction, Y_v is the vegetative productivity (g/m^2), λ_{Ei} is an empirical weathering constant (day^{-1}), t_e is the crop growth period (days) before harvest (by grazing in the case of pasture vegetation), and the deposition rate is in g/m^2-day. Based on a review of experimental values of r/Y_v for radionuclides, Chamberlain (1971) reports an average value of about 3.0 m^2/kg for grasses, based on a dry-weight value of Y_v of about 0.1 kg/m^2. The experiments providing a data base involved either the spraying of grasslands with nuclides dissolved in water or the use of 30 µm spores tagged with a nuclide. The USNRC Regulatory Guide suggests a value for r of 0.25 and a value for Y_v of 0.7 kg/m^2 fresh weight for depositing radionuclides on pasture. Neither of these literature sources relied on data obtained from organic chemicals applied or deposited on grasslands. It must be recognized that the amount of initial interception is a function of the exposed surface area of the vegetation, which may vary greatly within a species according to Y_v, and between species; the chemical and physical form of the compound depositing on the vegetation (i.e., in determining whether it is initially retained); and the presence of other vegetation which may interfere with interception by the species of concern. A default value for an interception fraction for TOX-SCREEN may be taken from some work of Morton et al. (1967) in which an interception of approximately 40% of applied herbicides was measured (Hoerger and Kenaga, 1972). This value of r may be more appropriate for organic chemicals than the Regulatory Guide value or Chamberlain's value, although a great deal of uncertainty still exists. A default value for Y_v might be 150 g/m^2, consistent with values reported by Chamberlain (1971) and Booth and Kaye (1971). The weathering constant, λ_{Ei}, is quite dependent on climatic factors, plant surface, exposed surface area, and the form of the compound. Although a value of 0.05 day^{-1}, corresponding to a 14 day half-life, is reported by Chamberlain and in the Regulatory Guide, a somewhat smaller value of λ_{Ei} is indicated for some organics (Hoerger and Kenaga, 1972). There is undoubtedly a large range in values of λ_{Ei} due to the variability in the factors affecting loss. It should be noted that λ_{Ei} does not include loss due to grazing.

The value of t_e will vary depending on grazing conditions, if a pasture is being considered. The value used in the Regulatory Guide is 30 days for grasses.

The total concentration in plants is calculated in TOX-SCREEN by summing concentrations due to root uptake and interception. As can be seen from the preceding discussion, there is a large uncertainty associated with these calculations due to the variability in parameters used. Because it is believed that grasslands would intercept depositing compounds to a greater degree than many other crops, based strictly on consideration of surface-to-volume ratios, it may be conservative to use parameter values pertinent to grasslands for all types of vegetation in estimating concentrations due to interception.

APPENDIX F
REFERENCES

1. Baes, C. F., III, "Prediction of Radionuclide K_D Values From Soil-Plant Concentration Ratios," *Trans. Am. Nucl. Soc.*, Vol. 38 (in press).

2. Booth, R. S. and S. V. Kaye, *A Preliminary Systems Analysis Model of Radioactivity Transfer to Man from Deposition in a Terrestrial Environment*, ORNL/TM-3135, Oak Ridge National Laboratory (1971).

3. Chamberlain, A. C., "Interception and Retention of Radioactive Aerosols by Vegetation," *Atmos. Environ*. 4:57-78 (1970).

4. Hoerger, F. and E. E. Kenaga, "Pesticide Residue on Plants: Correlation of Representative Data as a Basis for Estimation of Their Magnitude in the Environment," pp. 9-28 in *Global Aspects of Chemistry, Toxicology and Technology as Applied to the Environment*, Vol. I, F. Coulston and F. Korte, Eds., Academic Press, Inc., New York, New York (1972).

5. Karickoff, S. W., D. S. Brown, and T. A. Scott, "Sorption of Hydrophobic Pollutants on Natural Sediments," *Water Res*. 13: 241-248 (1979).

6. Mackay, D., "Correlation of Bioconcentration Factors," *Environ. Sci. Technol*. 16: 274-278 (1982).

7. McDowell-Boyer, L. M. and D. M. Hetrick, *A Multimedia Screening-Level Model for Assessing the Potential Fate of Chemicals Released to the Environment*, ORNL/TM-8334, Oak Ridge National Laboratory (1982).

8. Means, J. C., S. G. Wood, J. J. Hassett, and W. L. Banwart, "Sorption of Amino- and Carboxy-Substituted Polynuclear Aromatic Hydrocarbons by Sediments and Soils," *Environ. Sci. Technol*. 16: 93-98 (1982).

9. Morton, H. L., E. D. Robison, and R. E. Meyer, "Persistence of 2,4-D, 2,4,5-T, and Dicamba in Range Forage Grasses," *Weeds* 15: 268-271 (1967).

10. Neely, W. B., "Complex Problems - Simple Solutions," *Chemtech* 249-251 (April 1981).

11. Trabalka, J. R., Personal Communication, Oak Ridge National Laboratory, Oak Ridge, Tennessee (April 1982).

12. USNRC, Calculation of Annual Doses to Man From Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50, Appendix I, Regulatory Guide 1.109, Revision 1, Washington, D.C. (1977).